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On strict positive definiteness of product and product–sum covariance models

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Although positive definiteness is a sufficient condition for a function to be a covariance, the stronger strict positive definiteness is important for many applications, especially in spatial statistics, since it ensures that the kriging equations have a unique solution. In particular, spatial–temporal prediction has received a lot of attention, hence strictly positive definite spatial–temporal covariance models (or equivalently strictly conditionally negative definite variogram models) are needed.

In this paper the necessary and sufficient condition for the product and the product–sum space–time covariance models to be strictly positive definite (or the variogram function to be strictly conditionally negative definite) is given. In addition it is shown that an example appeared in the recent literature which purports to show that product–sum covariance functions may be only semi-definite is itself invalid. Strict positive definiteness of the sum of products model is also discussed.

1. Introduction

Fundamental results on positive definite (*p.d.*) functions were first given by Mathias (1923) and Schoenberg (1938a, 1938b). Bochner's (1959) Theorem not only provides the link between positive definiteness and covariance functions, but it also shows that p.d. functions have a unique spectral representation. The historical review of different forms of positive definiteness by Stewart (1976) is also worth noting.

In Geostatistics, many applications of p.d. functions pertain to spatial and spatial–temporal prediction. If the kriging equations are given in terms of the covariance function then strict positive definiteness is a sufficient condition for the existence of a unique solution of the kriging equations. When the kriging equations are given in terms of the variogram then strict conditional negative definiteness is sufficient to ensure a unique solution of the kriging equations. There have been a number of basic results pertaining to strict positive definiteness, even in numerical analysis including: Chang (1996), Strauss (1997) and zu Castell et al. (2005). The latter gave a sufficient condition for strict positive definiteness in $\mathbb{R}^d$. The result is based on the linear independence of the exponentials on sparse subsets.

Although there are examples in the literature where space–time covariance functions or space–time variograms are obtained by assuming that there is a suitable metric for space–time, time is not just another dimension. To ensure that time is treated differently it is useful to "separate" the dependence on spatial coordinates from the dependence on the temporal coordinate. The simplest example of a space–time covariance function is the product of a spatial covariance and

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a temporal covariance: this covariance function is called "separable" model or "product" model (Rodriguez-Iturbe and Meija, 1974; Posa, 1993; De Cesare et al., 1997). The assumption of separability for spatial and temporal processes offers a simplified representation of any variance–covariance matrix, and consequently, some remarkable computational benefits (Zimmerman, 1989; Genton, 2007). Separability is also an advantage when fitting a model to data; when re-written in variogram form, the separable model is characterized by its marginals. It is also important to underline that the product–sum model generalizes the product model and avoids some of the disadvantages of the separable model. The product and product–sum models (De Cesare et al., 2001a, 2001b; De Iaco et al., 2001), as well as the integrated product and integrated product–sum models (De Iaco et al., 2002a), are particularly advantageous because they can be used for more general non-geometric anisotropies. Thus, there is interest in whether the product, as well as the product–sum, of a strictly p.d. spatial covariance and a strictly p.d. temporal covariance is strictly p.d. in space–time. More generally, given a strictly p.d. covariance function defined on $\mathbb{R}^{\nu_1}$ and a second strictly p.d. covariance function defined on $\mathbb{R}^{\nu_2}$, the question is whether the product, as well as the product–sum, of the two factors is strictly p.d. on $\mathbb{R}^{\nu_1+\nu_2}$.

In this paper, Section 2 reviews some essential notions about second order stationary real valued random functions, product and product–sum models. Section 3 discusses a false counterexample regarding the product and product–sum models strict positive definiteness given in literature. Section 4 gives the necessary and sufficient condition for the product and the product–sum space–time covariance model to be strictly p.d. (or the variogram function to be strictly conditionally negative definite). Conditions for the strict positive definiteness of the more general sum of products model (Gregori et al., 2008) are also presented.

2. Basic notions

Let $Z(\mathbf{s},t)$ denote a second order stationary real valued random function, defined on $\mathbb{R}^d \times T$ ($d \in \mathrm{N}_+$), with covariance function given by

$$C_{ST}(\mathbf{h}_s,h_t) = Cov(Z(\mathbf{s}+\mathbf{h}_s,t+h_t),Z(\mathbf{s},t)),$$

where $\mathbf{h}_s$ and h_t are increments in space and time, respectively. Under the weaker assumption of intrinsic stationarity the variogram is given by

$$\gamma_{ST}(\mathbf{h}_s,h_t) = 0.5\,Var[Z(\mathbf{s}+\mathbf{h}_s,t+h_t)\quad Z(\mathbf{s},t)].$$

Assuming second order stationarity it is well known that the variogram and the covariance function are related:

$$\gamma_{ST}(\mathbf{h}_s,h_t) = C_{ST}(\mathbf{0},0)\quad C_{ST}(\mathbf{h}_s,h_t).$$

Two related functions are useful, called the *marginals* by analogy with marginals for probability density or probability distribution functions. $\gamma_{ST}(\mathbf{h}_s,0)$ and $\gamma_{ST}(\mathbf{0},h_t)$ are the spatial and temporal marginal variograms, respectively.

In the second order stationary case these can be written as $\gamma_{ST}(\mathbf{h}_s,0) = C_{ST}(0,0)\quad C_{ST}(\mathbf{h}_s,0)$ and $\gamma_{ST}(\mathbf{0},h_t) = C_{ST}(\mathbf{0},0)\quad C_{ST}(\mathbf{0},h_t)$. Recall that a real valued function $C_{ST}(\cdot)$ is p.d. on $\mathbb{R}^d \times T$ if for any $n \in N_+$ and any choice of $(\mathbf{s}_1,t_1),\ldots,(\mathbf{s}_n,t_n) \in \mathbb{R}^d \times T$ and $\lambda_1,\ldots,\lambda_n \in \mathbb{R}$ then

$$\sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j C_{ST}(\mathbf{s}_i\quad \mathbf{s}_j,t_i\quad t_j) Z\ 0. \tag{1}$$

The function $C_{ST}(\cdot)$ is *strictly p.d.*, if the above quadratic form is positive for any $n \in N_+$ and any choice of distinct points $(\mathbf{s}_1,t_1),\ldots,(\mathbf{s}_n,t_n) \in \mathbb{R}^d \times T$ and $\lambda_1,\ldots,\lambda_n \in \mathbb{R}$ not all zero.

While covariance functions need only be p.d., variograms need only be conditionally negative definite (*c.n.d.*), i.e.

$$\sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j \gamma_{ST}(\mathbf{s}_i\quad \mathbf{s}_j,t_i\quad t_j) \le 0, \tag{2}$$

for any $n \in N_+$ and any choice of $(\mathbf{s}_1,t_1),\ldots,(\mathbf{s}_n,t_n) \in \mathbb{R}^d \times T$ and $\lambda_1,\ldots,\lambda_n \in \mathbb{R}$ but with the restriction that

$$\sum_{i=1}^{n} \lambda_i = 0.$$

If the above quadratic form is negative for any choice of distinct points $(\mathbf{s}_1,t_1),\ldots,(\mathbf{s}_n,t_n) \in \mathbb{R}^d \times T$ and $\lambda_1,\ldots,\lambda_n \in \mathbb{R}$ not all zero, whose sum is zero, then the function $\gamma_{ST}(\cdot)$ is *strictly c.n.d.*

The earliest examples of space–time covariance models are either based on simplistic assumptions, i.e. they require the use of a metric in space–time or can result in p.d. as opposed to strictly p.d. functions. Geometric anisotropies can be incorporated via an affine transformation and space–time might be viewed as simply a higher dimensional space but possibly with an anisotropy in the model. This approach implies that there is an appropriate and natural choice of a norm (or metric) on space–time analogous to the usual Euclidean norm for space. The most obvious way to construct a model in space–time is to "separate" the dependence on space and on time. Early attempts used either the sum of two covariances (Rouhani and Hall, 1989) or the product of two covariances (Rodriguez-Iturbe and Meija, 1974; Posa, 1993; De Cesare et al., 1997), in either case one factor being defined on space and the other on time. It is easily shown that the sum model leads to p.d. (not strictly p.d.) models, hence the result may be a non-invertible kriging matrix (Myers and Journel, 1990). In the following, it is proved that the product of two strictly p.d. covariance functions in lower dimensional spaces is again a strictly p.d. covariance function in a higher dimensional space. Analogous results are also shown for the product-sum model.

2.1. Product and product–sum models

Let $Z_1(\mathbf{s})$ and $Z_2(t)$ be independent second order stationary random functions defined on $\mathbb{R}^d$ and T, respectively, with zero expected values and strictly p.d. covariance functions $C_S(\mathbf{h}_s)$ and $C_T(h_t)$. Then, the covariance function of $Z(\mathbf{s},t)=Z_1(\mathbf{s})Z_2(t)$ is

$$C_{ST}(\mathbf{h}_s,h_t)=C_S(\mathbf{h}_s)C_T(h_t). \tag{3}$$

In Section 4 it will be shown that C_{ST} is strictly p.d. on $\mathbb{R}^d\times T$ if and only if both factors, C_S and C_T, are strictly p.d. on $\mathbb{R}^d$ and T, respectively. However, the class (3) is severely limited, since each factor effectively must have the same "sill".

In variogram form the product model becomes

$$\gamma_{ST}(\mathbf{h}_s,h_t)=C_T(0)\gamma_S(\mathbf{h}_s)+C_S(\mathbf{0})\gamma_T(h_t)-\gamma_S(\mathbf{h}_s)\gamma_T(h_t) \tag{4}$$

or in terms of the marginals

$$\gamma_{ST}(\mathbf{h}_s,h_t)=\gamma_{ST}(\mathbf{h}_s,0)+\gamma_{ST}(\mathbf{0},h_t)-\frac{1}{C_T(0)C_S(\mathbf{0})}\gamma_{ST}(\mathbf{h}_s,0)\gamma_{ST}(\mathbf{0},h_t). \tag{5}$$

Some examples of the product covariance are given in De Cesare et al. (1997), as well as others.

A natural extension of the product model is the product–sum model. As introduced in De Cesare et al. (2001a, 2001b) and De Iaco et al. (2001), the product–sum covariance is given by

$$C_{ST}(\mathbf{h}_s,h_t)=k_1C_S(\mathbf{h}_s)C_T(h_t)+k_2C_S(\mathbf{h}_s)+k_3C_T(h_t), \tag{6}$$

with $k_1>0, k_2\geq 0, k_3\geq 0$. In Section 4 it will be shown that C_{ST} is strictly p.d. on $\mathbb{R}^d\times T$ if and only if both factors, C_S and C_T, are strictly p.d. on $\mathbb{R}^d$ and T, respectively.

This non-separable family of space–time covariances has been built by applying the convexity property of the covariances family (Matern, 1980).

Note that the product or sum model is easily obtained by the product–sum covariance model setting, respectively, $k_2=k_3=0$ or $k_1=0$.

The variogram form

$$\gamma_{ST}(\mathbf{h}_s,h_t)=[k_1C_T(0)+k_2]\gamma_S(\mathbf{h}_s)+[k_1C_S(\mathbf{0})+k_3]\gamma_T(h_t)-k_1\gamma_S(\mathbf{h}_s)\gamma_T(h_t) \tag{7}$$

or

$$\gamma_{ST}(\mathbf{h}_s,h_t)=\gamma_{ST}(\mathbf{h}_s,0)+\gamma_{ST}(\mathbf{0},h_t)-k\gamma_{ST}(\mathbf{h}_s,0)\gamma_{ST}(\mathbf{0},h_t) \tag{8}$$

is somewhat more convenient.

As shown in De Iaco et al. (2001), this last spatial temporal variogram is c.n.d. if and only if the following condition for the parameter k is satisfied:

$$0<k\leq\frac{1}{\max\{\text{sill }\gamma_{ST}(\mathbf{h}_s,0),\text{sill }\gamma_{ST}(\mathbf{0},h_t)\}}. \tag{9}$$

Some applications are found in De Iaco et al. (2000, 2002b).

3. A misleading counterexample

In Gregori et al. (2008) it is claimed that the product–sum model is not strictly p.d. for some choices of strictly p.d. marginals in some pathological situations. Their purported counterexample uses the variogram form of the product–sum model (De Iaco et al., 2001) but in two-dimensional space instead of space time. They give it as

$$\gamma(x,y)=\gamma_{1s}(x,0)+\gamma_{2s}(0,y)-k\gamma_{1s}(x,0)\gamma_{2s}(0,y). \tag{10}$$

As noted above this is the variogram form of Eq. (6), i.e. the marginals correspond to covariance functions defined on one-dimensional space. If these covariance functions are strictly p.d. then the product–sum covariance function is strictly p.d. on two-dimensional space if $k_1>0$ and $k_2,k_3\geq 0$. De Iaco et al. (2001) show that these inequalities are satisfied if and only if condition (9) is satisfied. In turn with these conditions and strictly p.d. covariance functions the space time covariance function in Eq. (6) is strictly p.d. or equivalently, the variogram in Eq. (10) is strictly c.n.d. when the marginal variograms are strictly c.n.d. In quoting this theorem and in their example Gregori et al. (2008) neglect the strict positive definiteness (strict conditional negative definiteness for variograms).

Although the model is given in terms of variograms, second order stationarity is assumed and hence each variogram corresponds to a covariance function.

The example given in Gregori et al. (2008) considered four data points $\{\mathbf{u}_1=(0,0),\ \mathbf{u}_2=(a,0),\ \mathbf{u}_3=(0,b),\ \mathbf{u}_4=(a,b)\}$ with variogram values $\gamma_{1s}(a,0)=c$, $\gamma_{2s}(0,b)=d$ with $c=d/(d-1)$ and $d>1$ and $sill[\gamma_{1s}(x,0)]=sill[\gamma_{2s}(x,0)]=1$ with $k=1$.

First of all, the values chosen for the marginal sills and the k parameter, imply that (10) is actually the variogram form of the product of two covariance functions and hence the global sill $C(0,0)$ is also equal to 1. In turn this implies that:

1. $|C(x,y)|\le 1$,
2. $0\le\gamma(x,y)\le 2$.

Obviously, the same inequalities hold for the marginals.

Secondly, the values they assigned to the variogram marginals contradict the inequalities in 1 and 2 for $d\in]1,2[\cup]2,+\infty[$, since $\gamma(a,0)=d/(d-1)>2$ for $1<d<2$, $\gamma(0,b)=d>2$ for $d>2$. If $d=2$ then $c=d=\gamma(a,0)=\gamma(0,b)$ and $C(a,0)=C(0,b)=-1$. In this case, the marginals are not strictly p.d., as easily shown in the following example.

Let $\mathbf{u}_1=(0,0)$, $\mathbf{u}_2=(0,b)$ be two points in $\mathbb{R}^2$ and $\lambda_1=\lambda_2=1$, then

$$\sum_{i=1}^{2}\sum_{j=1}^{2}\lambda_i\lambda_j C_1(x_i-x_j)\cdot C_2(y_i-y_j)=2C(0,0)+2C(0,b)=0.$$

Thus the marginal covariance C_2 is not strictly p.d. Similarly for the marginal covariance C_1.

Hence, when it is assumed that $C(a,0)=C(0,b)=-1$, it is not surprising if the covariance kriging matrix might be singular in some cases (Dimitrakopoulos and Luo, 1994).

It is well known that strict positive definiteness of the spatial and temporal marginals is a necessary condition for a space–time model to be strictly p.d. If the spatial and temporal marginals are not both strictly p.d., then the model is not strictly p.d. In the following, it is shown that strict positive definiteness of both factors in (3) is a necessary as well as a sufficient condition for the product of two covariance functions to be strictly p.d.

Alternatively to the previous argumentation, it can be shown that the values given to the variogram marginals produce a variogram matrix which is not c.n.d.

Proof. Compute the quadratic form for the given four data points as follows:

$$\sum_{i=1}^{4}\sum_{j=1}^{4}\lambda_i\lambda_j\gamma(\mathbf{u}_i-\mathbf{u}_j)=[\lambda_1^2+\lambda_2^2+\lambda_3^2+\lambda_4^2]\cdot 0+[2\lambda_1\lambda_2+2\lambda_3\lambda_4]\cdot\frac{d}{d-1}+[2\lambda_1\lambda_3+2\lambda_2\lambda_4]\cdot d+[2\lambda_1\lambda_4+2\lambda_2\lambda_3]\cdot 0.$$

Let λ be a non-zero real number and K any real number; then setting $\lambda_1=-K\lambda,\lambda_2=-\lambda,\lambda_3=K\lambda,\lambda_4=\lambda$, the quadratic form becomes

$$[4K\lambda^2]\frac{d}{d-1}+[-2K^2\lambda^2-2\lambda^2]d=2\lambda^2\frac{d}{d-1}[2K-(K^2+1)(d-1)].$$

It is easy to show that for any $1<d<2$, there is a K such that the factor in brackets is greater than 0, thus the double sum is greater than 0 and the function is not c.n.d. □

4. Strict positive definiteness

Strict positive definiteness is important for space–time covariance models, because it ensures the invertibility of the matrices involved in most of the interpolation procedures (e.g. the coefficient matrix in the kriging equations).

In the following, it is shown that the product and the product–sum models of two strictly p.d. covariances, defined on two different sub-spaces (for example, spatial and temporal domains), are again strictly p.d. This result is implicit in Strauss (1997) but not explicit and there it requires the Hilbert space setting using reproducing kernels.

4.1. Strict positive definiteness of product covariance functions

Theorem 1. *Let C_1 and C_2 be second order stationary covariance functions, defined on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$ ($\nu_1,\nu_2\in\mathrm{N}_+$, $\nu_1+\nu_2=\nu$), respectively, and*

$$C(\mathbf{h})=C(\mathbf{h}_1,\mathbf{h}_2)=C_1(\mathbf{h}_1)C_2(\mathbf{h}_2),\quad \mathbf{h}_1\in\mathbb{R}^{\nu_1},\ \mathbf{h}_2\in\mathbb{R}^{\nu_2} \tag{11}$$

be a second order stationary covariance function defined on $\mathbb{R}^{\nu}$. C is a strictly p.d. covariance on $\mathbb{R}^{\nu}$ if and only if C_1 and C_2 are two strictly p.d. covariances, defined on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$ ($\nu_1,\nu_2\in\mathrm{N}_+$, $\nu_1+\nu_2=\nu$), respectively.

Proof. Part 1 (only if) If the covariance function C in (11) is a strictly p.d., then for any $n\in N_+$ and any choice of $\mathbf{u}_1=(\mathbf{x}_1,\mathbf{y}_1),\ldots,\mathbf{u}_n=(\mathbf{x}_n,\mathbf{y}_n)\in\mathbb{R}^{\nu_1}\times\mathbb{R}^{\nu_2}$ and $\lambda_1,\ldots,\lambda_n\in\mathbb{R}$ not all zero,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j C_1(\mathbf{x}_i-\mathbf{x}_j)C_2(\mathbf{y}_i-\mathbf{y}_j)>0. \tag{12}$$

This implies that for any $n \in N_+$ and any choice of $\mathbf{u}_1 = (\mathbf{x}_1,\mathbf{y}_1),\ldots,\mathbf{u}_n = (\mathbf{x}_n,\mathbf{y}_n) \in \mathbb{R}^{\nu_1} \times \mathbb{R}^{\nu_2}$, where $\mathbf{y}_1 = \cdots = \mathbf{y}_n$, and $\lambda_1,\ldots,\lambda_n \in \mathbb{R}$ not all zero,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j C_1(\mathbf{x}_i - \mathbf{x}_j)C_2(\mathbf{0}) = C_2(\mathbf{0})\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j C_1(\mathbf{x}_i - \mathbf{x}_j) > 0.$$

Hence

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j C_1(\mathbf{x}_i - \mathbf{x}_j) > 0.$$

Thus C_1 is strictly p.d. Similarly, for any $n \in N_+$ and any choice of $\mathbf{u}_1 = (\mathbf{x}_1,\mathbf{y}_1),\ldots,\mathbf{u}_n = (\mathbf{x}_n,\mathbf{y}_n) \in \mathbb{R}^{\nu_1} \times \mathbb{R}^{\nu_2}$, where $\mathbf{x}_1 = \cdots = \mathbf{x}_n$, and $\lambda_1,\ldots,\lambda_n \in \mathbb{R}$ not all zero,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j C_1(\mathbf{0})C_2(\mathbf{y}_i - \mathbf{y}_j) = C_1(\mathbf{0})\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j C_2(\mathbf{y}_i - \mathbf{y}_j) > 0.$$

Hence

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j C_2(\mathbf{y}_i - \mathbf{y}_j) > 0,$$

thus C_2 is strictly p.d.

Part 2 (if). Second part (from right to left) of the proof follows.

Let $\mathbf{u}_1=(\mathbf{x}_1,\mathbf{y}_1)$, $\mathbf{u}_2=(\mathbf{x}_2,\mathbf{y}_2),\ldots,\mathbf{u}_n=(\mathbf{x}_n,\mathbf{y}_n)$ be distinct points in $\mathbb{R}^{\nu_1} \times \mathbb{R}^{\nu_2}$, let $\mathbf{x}_1,\ldots,\mathbf{x}_{n_1}$ and $\mathbf{y}_1,\ldots,\mathbf{y}_{n_2}$ be the corresponding distinct coordinates in $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$, respectively. Then $\{\mathbf{u}_1,\ldots,\mathbf{u}_n\}$ is a subset of $\{(\mathbf{x}_i,\mathbf{y}_k) \in \mathbb{R}^{\nu_1} \times \mathbb{R}^{\nu_2}, i = 1,\ldots,n_1, k = 1,\ldots,n_2\}$. The latter set is an $(n_1 \times n_2)$ regular pattern.

Let Σ be the $N \times N$ matrix, where $N=n_1 \times n_2$, whose entries are $C(\mathbf{x}_i - \mathbf{x}_j,\mathbf{y}_k - \mathbf{y}_l)$, $i,j=1,2,\ldots,n_1$, $k,l=1,2,\ldots,n_2$.

Because C in (11) is a product, i.e. separable, the covariance matrix Σ can be written as the Kronecker product of two smaller matrices $\mathbf{C}_{1(n_1 \times n_1)}$ and $\mathbf{C}_{2(n_2 \times n_2)}$:

$$\Sigma = \mathbf{C}_1 \otimes \mathbf{C}_2, \tag{13}$$

where the generic element of $\mathbf{C}_1$ is $C_1(\mathbf{x}_i - \mathbf{x}_j)$, $i,j=1,2,\ldots,n_1$ and the generic element of $\mathbf{C}_2$ is $C_2(\mathbf{y}_k - \mathbf{y}_l)$, $k,l=1,2,\ldots,n_2$.

If C_1 and C_2 are two strictly p.d. second order stationary covariances on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$, respectively, then their eigenvalues $\alpha_1,\alpha_2,\ldots,\alpha_{n_1}$ and $\beta_1,\beta_2,\ldots,\beta_{n_2}$, respectively, are all positive. Hence, the eigenvalues of the Kronecker product Σ are all positive, since they are obtained as the product $\alpha_i\beta_j$, $i=1,2,\ldots,n_1$, $j=1,2,\ldots,n_2$ (Graham, 1981).

This means that the $(n_1 \times n_2) \times (n_1 \times n_2)$ matrix of product covariances corresponding to the $(n_1 \times n_2)$ regular pattern in $\mathbb{R}^{\nu_1} \times \mathbb{R}^{\nu_2}$ is always strictly p.d.:

$$\sum_{i=1}^{n_1}\sum_{j=1}^{n_1}\sum_{k=1}^{n_2}\sum_{l=1}^{n_2}\lambda_{ik}\lambda_{jl}C(\mathbf{x}_i - \mathbf{x}_j,\mathbf{y}_k - \mathbf{y}_l) > 0, \tag{14}$$

for all choices of the coefficients not all zero.

Recall that a symmetric matrix is strictly p.d. if all only if the leading principal minors are positive, then it can be shown that the leading principal minors of the $(n \times n)$ matrix of a product covariance function, corresponding to the subset $\mathbf{u}_1, \mathbf{u}_2,\ldots,\mathbf{u}_n$, are also positive. This implies that the covariance matrix of the product of two strictly p.d. functions is strictly p.d. □

Thus strict positive definiteness of both factors is a necessary as well as a sufficient condition for the product of two covariance functions to be strictly p.d.

A simple example illustrates how any choice of n points in $\mathbb{R}^{\nu_1} \times \mathbb{R}^{\nu_2}$ can be viewed as a subset of a regular configuration.

Let $\{\mathbf{u}_1,\mathbf{u}_2,\mathbf{u}_3\}$ be three points in $\mathbb{R}^2$, where x_1,x_2,x_3 and y_1,y_2,y_3 are the corresponding distinct coordinates on $\mathbb{R}$. Fig. 1 illustrates how the three points would appear as a subset of the regular pattern.

The strict positive definiteness of the more general sum of products model proposed by Gregori et al. (2008) can be also guaranteed. In Gregori et al. (2008), the general sum of products model is defined as follows.

Let $\{C_{1i}:i=1,\ldots,n\}$ and $\{C_{2i}:i=1,\ldots,n\}$, $n \in \mathrm{N}$, be, respectively, valid continuous and integrable covariance functions defined on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$ ($\nu_1,\nu_2 \in \mathrm{N}_+$, $\nu_1+\nu_2=\nu$), and let f_{1i} and f_{2i}, $i=1,\ldots,n$, be the Fourier transforms of covariances C_{1i} and C_{2i}, respectively. Assume that at least one couple of Fourier transforms, say (f_{1n},f_{2n}), is composed of non-vanishing functions, so that the following quantities are defined:

$$m_{1i} := \inf_{\mathbf{x}\in\mathbb{R}^{\nu_1}}\frac{f_{1i}(\mathbf{x})}{f_{1n}(\mathbf{x})},\quad M_{1i} := \sup_{\mathbf{x}\in\mathbb{R}^{\nu_1}}\frac{f_{1i}(\mathbf{x})}{f_{1n}(\mathbf{x})},\quad m_{2i} := \inf_{\mathbf{y}\in\mathbb{R}^{\nu_2}}\frac{f_{2i}(\mathbf{y})}{f_{2n}(\mathbf{y})},\quad M_{2i} := \sup_{\mathbf{y}\in\mathbb{R}^{d_2}}\frac{f_{2i}(\mathbf{y})}{f_{2n}(\mathbf{y})}.$$

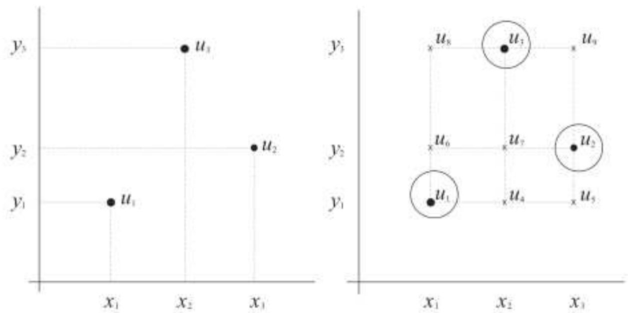

Fig. 1. (a) Data points; (b) regular pattern.

For $k_1,\ldots,k_n \in \mathbb{R}$, consider the following model:

$$C(\mathbf{h}_1,\mathbf{h}_2) = \sum_{i=1}^{n} k_i C_{1i}(\mathbf{h}_1) C_{2i}(\mathbf{h}_2), \quad \mathbf{h}_1 \in \mathbb{R}^{\nu_1}, \ \mathbf{h}_2 \in \mathbb{R}^{\nu_2}, \tag{15}$$

then

1. if model (15) is p.d., then the coefficient k_n must satisfy the following condition:

$$k_n \, \mathrm{Z} \quad \sum_{i=1}^{n-1} k_i [M_{1i} M_{2i} \mathbf{1}_{\{k_i \, \mathrm{Z} \, 0\}} + m_{1i} m_{2i} \mathbf{1}_{\{k_i < 0\}}]; \tag{16}$$

2. if the coefficient k_n satisfies the following condition:

$$k_n \, \mathrm{Z} \quad \sum_{i=1}^{n-1} k_i [m_{1i} m_{2i} \mathbf{1}_{\{k_i \, \mathrm{Z} \, 0\}} + M_{1i} M_{2i} \mathbf{1}_{\{k_i < 0\}}], \tag{17}$$

then model (15) is p.d.

Note that this model is a special case of a sum of products (of pairs of covariance functions) and in turn is a special case of an integrated product sum model as in De Iaco et al. (2002a).

Theorem 2. *Given the model* (15) *for* C , *if* C_{1i} *and* C_{2i}, $i=1,\mathrm{y} \ ,n$, *are continuous and absolutely integrable covariance functions defined, respectively, on* $\mathbb{R}^{\nu_1}$ *and* $\mathbb{R}^{\nu_2}$, *with* $\nu_1,\nu_2 \in \mathrm{N}_+$, $\nu_1+\nu_2=\nu$, *with at least one pair of non-vanishing Fourier transforms, say* (f_{1n},f_{2n}), *and*

$$k_n \, 4 \quad \sum_{i=1}^{n-1} k_i \frac{C_{1i}(\mathbf{0}) C_{2i}(\mathbf{0})}{C_{1n}(\mathbf{0}) C_{2n}(\mathbf{0})}, \tag{18}$$

so that the function C *is not identically zero* (*it is positive at zero*), *then*

1. *if model* (15) *is strictly p.d., then the admissible values for the coefficient* k_n *must satisfy condition* (16);
2. *if the coefficient* k_n *satisfies condition* (17), *then model* (15) *is strictly p.d.*

Proof. Since C_{1i} and C_{2i}, $i=1,\mathrm{y} \ ,n$, are supposed to be continuous and absolutely integrable covariance functions defined, respectively, on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$, with $\nu_1,\nu_2 \in \mathrm{N}_+$, $\nu_1+\nu_2=\nu$, then the general sum of products model C is continuous and absolutely integrable. Moreover, the general sum of products model C is bounded, since C_{1i} and C_{2i}, $i=1,\mathrm{y} \ ,n$, are bounded.

Now, recall that, given a continuous and absolutely integrable function C, then C is strictly p.d. if and only if C is bounded and its Fourier transform is non-negative and non-vanishing (Chang, 1996; Wendland, 2005).

Hence, if C is strictly p.d., then the Fourier transform of model (15)

$$f(\mathbf{x},\mathbf{y}) = \sum_{i=1}^{n} k_i f_{1i}(\mathbf{x}) f_{2i}(\mathbf{y})$$

is non-negative, consequently the coefficient k_n has to satisfy condition (16), as proved in Gregori et al. (2008). It is well known that it suffices to show that the Fourier transform is non-negative when the function C is not the zero function, because then the Fourier transform cannot vanish. The function C is not the zero function under the condition (18) on k_n.

If the coefficient k_n satisfies the conditions (17) and (18), the Fourier transform $f(\mathbf{x},\mathbf{y})$ of model (15) is non-negative, as shown in Gregori et al. (2008), and non-vanishing, since the function C is not the zero function, then C is strictly p.d. $\square$

4.2. The strict positive definiteness of product–sum models

Theorem 3. *Let C_1 and C_2 be second order stationary covariance functions, defined on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$ $(\nu_1,\nu_2 \in \mathrm{N}_+,\ \nu_1+\nu_2=\nu)$, respectively, and*

$$C(\mathbf{h}) = C(\mathbf{h}_1,\mathbf{h}_2) = k_1 C_1(\mathbf{h}_1)C_2(\mathbf{h}_2) + k_2 C_1(\mathbf{h}_1) + k_3 C_2(\mathbf{h}_2), \quad \mathbf{h}_1 \in \mathbb{R}^{\nu_1},\ \mathbf{h}_2 \in \mathbb{R}^{\nu_2} \tag{19}$$

be a second order stationary covariance defined on $\mathbb{R}^{\nu}$, where $k_1 > 0, k_2 \geq 0, k_3 \geq 0$ are real constants. C is a strictly p.d. covariance on $\mathbb{R}^{\nu}$ if and only if C_1 and C_2 are two strictly p.d. covariances, defined on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$ $(\nu_1,\nu_2 \in \mathrm{N}_+,\ \nu_1+\nu_2=\nu)$, respectively.

Proof. In the following proofs, k_2 and k_3 are assumed to be greater than zero, since for $k_2=k_3=0$ the product–sum model reduces to the product model, for which analogous results have been proved in the previous paragraph.

Part 1 (only if). Assume ab absurdo that one of the marginal covariances, that is C_1, is only p.d., then

$$\sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j k_1[C_1(\mathbf{x}_i-\mathbf{x}_j)C_2(\mathbf{y}_i-\mathbf{y}_j)] \geq 0; \tag{20}$$

hence, recall that the sum of two covariance functions defined on two different sub-spaces is only p.d. (Myers and Journel, 1990), that is

$$\sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j [k_2 C_1(\mathbf{x}_i-\mathbf{x}_j)+k_3 C_2(\mathbf{y}_i-\mathbf{y}_j)] \geq 0, \tag{21}$$

consequently, the sum of two p.d. covariances, that is (20) and (21), is only p.d. (Wendland, 2005).

As a consequence of above, the strictly positive definiteness hypothesis on C is not compatible.

Part 2 (if). Recall that the product–sum model is given by the sum of

- a strictly p.d. function on $\mathbb{R}^{\nu}$, corresponding to the product of two strictly p.d. functions defined on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$, where $\nu=\nu_1+\nu_2$,
- a p.d. function on $\mathbb{R}^{\nu}$, corresponding to the sum of two strictly p.d. functions defined on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$.

The proof follows by noting that the product of two strictly p.d. functions defined on $\mathbb{R}^{\nu_1}$ and $\mathbb{R}^{\nu_2}$ is strictly p.d. on the product space $\mathbb{R}^{\nu}$, and the sum of a strictly p.d. function on $\mathbb{R}^{\nu}$ and a p.d. function on the same space is again strictly p.d. on $\mathbb{R}^{\nu}$, that is

$$\underbrace{\sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j k_1 C_1(\mathbf{x}_i-\mathbf{x}_j)C_2(\mathbf{y}_i-\mathbf{y}_j)}_{>0} + \underbrace{\sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j [k_2 C_1(\mathbf{x}_i-\mathbf{x}_j)+k_3 C_2(\mathbf{y}_i-\mathbf{y}_j)]}_{\geq 0}$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j [k_1 C_1(\mathbf{x}_i-\mathbf{x}_j)C_2(\mathbf{y}_i-\mathbf{y}_j)+k_2 C_1(\mathbf{x}_i-\mathbf{x}_j)+k_3 C_2(\mathbf{y}_i-\mathbf{y}_j)] > 0. \quad \square$$

Corollary 1. *The variogram form (7) or (8) of the product–sum covariance function is strictly c.n.d. if and only if the corresponding marginals are strictly c.n.d.*

The following examples highlight how the product–sum model might be viewed as a generalization of the product model. Exponential and Gaussian models are considered, since they are widely used as marginals in the product–sum model in different areas, ranging from environmental sciences to medicine, from ecology to hydrology; some applications are found in De Iaco et al. (2000, 2002b), Myers (2002), Fernandez-Casal et al. (2003), Gething et al. (2006), Skien and Blöschl (2006), Spadavecchia and Williams (2009), De Iaco (2010), among others.

Example 1. There are two different exponential covariance function models, one of which is the product to two exponential models of the same type (or more depending on the dimension of the space) (Dimitrakopoulos and Luo, 1994), that is

$$C(\mathbf{h}_1,\mathbf{h}_2) = \exp(-a|\mathbf{h}_1|-b|\mathbf{h}_2|) = \exp(-a|\mathbf{h}_1|)\exp(-b|\mathbf{h}_2|) = C_1(\mathbf{h}_1)C_2(\mathbf{h}_2).$$

This model is a special case of the product model, i.e. given two valid covariance functions, the product is again a valid model.

In variogram form this becomes

$$\gamma(\mathbf{h}_1,\mathbf{h}_2)=1-\exp(-a\|\mathbf{h}_1\|-b\|\mathbf{h}_2\|).$$

Using the product–sum form this can be generalized to

$$\gamma(\mathbf{h}_1,\mathbf{h}_2)=[1-\exp(-a\|\mathbf{h}_1\|)]+[1-\exp(-a\|\mathbf{h}_2\|)]-k[1-\exp(-a\|\mathbf{h}_1\|)][1-\exp(-b\|\mathbf{h}_2\|)]. \tag{22}$$

If $k=1$ then the model is just the exponential variogram model. If $0<k<1$ the variogram is anisotropic but it is not a geometric anisotropy.

Example 2. The Gaussian covariance function can be written as follows:

$$C(\mathbf{h}_1,\mathbf{h}_2)=\exp(-a\|\mathbf{h}_1\|^2-b\|\mathbf{h}_2\|^2)=\exp(-a\|\mathbf{h}_1\|^2)\cdot\exp(-b\|\mathbf{h}_2\|^2)=C_1(\mathbf{h}_1)C_2(\mathbf{h}_2).$$

In variogram form this becomes

$$\gamma(\mathbf{h}_1,\mathbf{h}_2)=1-\exp(-a\|\mathbf{h}_1\|^2-a\|\mathbf{h}_2\|^2).$$

This might be generalized to

$$\gamma(\mathbf{h}_1,\mathbf{h}_2)=[1-\exp(-a\|\mathbf{h}_1\|^2)]+[1-\exp(-b\|\mathbf{h}_2\|^2)]-k[1-\exp(-a\|\mathbf{h}_1\|^2)][1-\exp(-b\|\mathbf{h}_2\|^2)],$$

which reduces to the usual Gaussian model if $k=1$.

Additional spatial models with zonal anisotropies can be found in Myers (2008).

5. Summary

While covariance functions need only be p.d. and variograms need only be c.n.d., these conditions are not sufficient to ensure that the kriging equations have a unique solution. Instead strict positive definiteness is sufficient for covariance functions and strict conditionally negative definiteness is sufficient for variograms. To ensure that the product and the product–sum space–time covariance functions are strictly p.d. (or that the corresponding variogram models are strictly c.n.d.), it is shown that it is necessary and sufficient that the marginal covariance functions be strictly p.d. (or the marginal variograms be strictly c.n.d.). This shows that the claim made by Gregori et al. (2008) is not true; it is also proved that the purported counterexample given in that paper is not a variogram because it is not c.n.d. Moreover, the strict positive definiteness of the sum of products model proposed by Gregori et al. (2008) can be also guaranteed under specific conditions on both the marginals and the coefficients.

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