Space-time analysis using a general product-sum model

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Abstract

A generalization of the product-sum covariance model introduced by De Cesare et al. (2001) is given in this paper. This generalized model is non-separable and in general is non-integrable, hence it cannot be obtained from the Cressie-Huang representation. Moreover, the product-sum model does not correspond to the use of a metric in space-time. It is shown that there are simple methods for estimating and modeling the covariance or variogram components of the product-sum model using data from realizations of spatial-temporal random fields.

Keywords: Space-time random fields.

1 Introduction

There are two main difficulties in modeling spatial-temporal correlation, the first being how to ensure that one has a valid model, the second being how to fit the data to the model. The earliest examples of models are either based on simplistic assumptions, e.g. require the use of a metric in space-time, or can lead to semi-definite as opposed to positive definite functions. A product model was used in De Cesare et al. (1997) which was then extended to a product-sum model (De Cesare et al., 2001). In Cressie and Huang (1999) it was shown that the product model is essentially a special case of a product-integral model. For each of these model constructions it is necessary to fit a function which depends on the spatial component and a function which depends on the temporal component. The results presented subsequently address both of the questions above. The generalized product-sum model provides a large new class of models not obtainable from the Cressie-Huang representation and which are easily modeled using techniques similar to those used for modeling spatial variograms. De Cesare et al. (2001) includes a brief comparison of the (simplified) product-sum covariance model and some other classes of spatial-temporal covariance models that have appeared in the literature. These include the metric model (Dimitrakopoulos and Luo, 1994), the product model (Rodriguez-Iturbe and Meija, 1974), the linear model (Rouhani and Hall, 1989), the product model (De Cesare et al., 1997) and the integrated product model (Cressie and Huang, 1999). In that paper, two simplifying constraints were imposed on the coefficients in the product sum model. These constraints were used to ensure the positive definiteness property and to simplify estimating the coefficients, i.e., fitting the model to the data. These constraints are replaced by a more general set of conditions in this paper.

This leads to aa more general class of the product-sum covariance models (as well as the corresponding variogram models). Moreover it is shown that, after modeling the spatial and temporal components, the spatial-temporal variogram function depends on only one parameter, which has to be estimated from data. Admissible values for this parameter are dependent on the sill values of the spatial-temporal component variograms. This leads to a necessary and sufficient condition for positive definiteness, i.e., conditional negative definiteness for the variogram form. Practical aspects for fitting the spatial-temporal variogram to data are discussed.

2 A generalization of the product-sum model

Let $Z = \{Z(s,t), (s,t) \in D \times T\}$ be a second order stationary spatial-temporal random field, where $D \subset \Re^d$ and $T \subset \Re_+$, with expected value, covariance and variogram, respectively:

$$E(Z(s,t)) = 0,$$

$$C_{s,t}(h_s, h_t) = Cov(Z(s+h_s, t+h_t), Z(s,t)), \tag{1}$$

$$\gamma_{s,t}(h_s, h_t) = \frac{Var(Z(s+h_s, t+h_t) - Z(s,t))}{2},$$

where $(s, s+h_s) \in D^2$ and $(t, t+h_t) \in T^2$.

The function $C_{s,t}$ in (1) must satisfy a positive-definiteness condition in order to be an admissible covariance model. That is, for any $(s_i, t_j) \in D \times T$, any $a_{ij} \in \Re, i = 1, \ldots, n_s, j = 1, \ldots, n_t$, and any positive integers n_s and n_t, $C_{s,t}$ must satisfy:

$$\sum_{i=1}^{n_s} \sum_{j=1}^{n_t} \sum_{k=1}^{n_s} \sum_{l=1}^{n_t} a_{ij} a_{kl} C_{s,t}(s_i - s_k, t_j - t_l) \geq 0.$$

The following class of valid product-sum covariance models was introduced in De Cesare et al. (2001):

$$C_{s,t}(h_s, h_t) = k_1 C_s(h_s) C_t(h_t) + k_2 C_s(h_s) + k_3 C_t(h_t), \tag{2}$$

where C_t and C_s are valid temporal and spatial covariance models, respectively. For positive definiteness it is then sufficient that $k_1 > 0, k_2 \geq 0$ and $k_3 \geq 0$. In De Cesare et al. (2001) two simplifying assumptions were made, but these last will be replaced by more general conditions. The above model can be also written in terms of the variograms :

$$\gamma_{s,t}(h_s, h_t) = (k_2 + k_1 C_t(0))\gamma_s(h_s) + (k_3 + k_1 C_s(0))\gamma_t(h_t) - k_1 \gamma_s(h_s)\gamma_t(h_t), \tag{3}$$

where γ_s and γ_t are valid spatial and temporal variogram models, while $C_s(0)$ and $C_t(0)$ are the corresponding sill values. The second-order stationarity assumption is sufficient to ensure that these variograms have sills, i.e. they are asymptotically bounded.
Using the defining property, $\gamma(0) = 0$, it follows that :

$$\gamma_{s,t}(h_s, 0) = (k_2 + k_1 C_t(0))\gamma_s(h_s) = k_s \gamma_s(h_s), \tag{4}$$

and

$$\gamma_{s,t}(0, h_t) = (k_3 + k_1 C_s(0))\gamma_t(h_t) = k_t \gamma_t(h_t), \tag{5}$$

where k_s and k_t can be viewed as coefficients of proportionality between the space-time variograms $\gamma_{s,t}(h_s, 0)$ and $\gamma_{s,t}(0, h_t)$ and the spatial and temporal variogram models $\gamma_s(h_s)$ and $\gamma_t(h_t)$, respectively. k_s and k_t were both assumed to be one in De Cesare et al. (2001). This was in order to simplify fitting the model, i.e., determining k_1, k_2 and k_3. However as will now be shown, those restrictions are not necessary and impose a form of unnecessary symmetry on the model, i.e., symmetry between the impact of the spatial correlation component and the temporal correlation component. First it is shown that all three coefficients in the model can be written in terms of the sills and the two parameters k_s and k_t. In particular this will lead to modeling $\gamma_s(h_s)$ and $\gamma_t(h_t)$ by modeling $\gamma_{s,t}(h_s, 0)$ and $\gamma_{s,t}(0, h_t)$, respectively. Then these two parameters will be combined into a single parameter in the model.
Combining:

$$(k_2 + k_1 C_t(0)) = k_s,$$

$$(k_3 + k_1 C_s(0)) = k_t,$$

obtained from (4) and (5), along with

$$C_{s,t}(0, 0) = k_1 C_s(0) C_t(0) + k_2 C_s(0) + k_3 C_t(0),$$

obtained from (2). The coefficients k_1, k_2 and k_3 can be solved for in terms of the sill values $C_{s,t}(0,0), C_s(0)$, $C_t(0)$ and the parameters k_s, k_t:

$$k_1 = \frac{k_s C_s(0) + k_t C_t(0) - C_{s,t}(0,0)}{C_s(0)C_t(0)}, \tag{6}$$

$$k_2 = \frac{C_{s,t}(0,0) - k_t C_t(0)}{C_s(0)}, \tag{7}$$

$$k_3 = \frac{C_{s,t}(0,0) - k_s C_s(0)}{C_t(0)}. \tag{8}$$

Since for positive definiteness $k_1 > 0, k_2 \geq 0$ and $k_3 \geq 0$, admissibility for the class of covariance models (and the corresponding class of product-sum variogram models) defined in (2) is related to the sills of the spatial and temporal components.

3 Some general results

The product-sum model exhibits several interesting and perhaps unexpected features involving the sill values of the component variograms. Using the link between a variogram and the corresponding covariance, it follows that:

$$\gamma_{s,t}(h_s, h_t) = C_{s,t}(0,0) - C_{s,t}(h_s, h_t), \tag{9}$$

$$\gamma_{s,t}(h_s, 0) = C_{s,t}(0,0) - C_{s,t}(h_s, 0), \tag{10}$$

and

$$\gamma_{s,t}(0, h_t) = C_{s,t}(0,0) - C_{s,t}(0, h_t). \tag{11}$$

By examining the asymptotic behaviour of $\gamma_{s,t}(h_s, h_t)$, $\gamma_{s,t}(h_s, 0)$ and $\gamma_{s,t}(0, h_t)$, the following theorem shows that these variograms do not reach the same sill value.

Theorem 1 *Let Z be a second order stationary spatial-temporal random field. Assume that the space-time covariance $C_{s,t}$ has the form given in (2) and suppose that $C_{s,t}$ is continuous in space-time. Then using (4) and (5), the following are obtained:*

$$\lim_{h_s \to \infty} \lim_{h_t \to \infty} \gamma_{s,t}(h_s, h_t) = C_{s,t}(0,0), \tag{12}$$

$$\lim_{h_s \to \infty} \gamma_{s,t}(h_s, 0) = k_s C_s(0), \tag{13}$$

$$\lim_{h_t \to \infty} \gamma_{s,t}(0, h_t) = k_t C_t(0). \tag{14}$$

Proof. In order to prove (12), it is sufficient to recall the continuity of $C_{s,t}$:

$$\lim_{h_s\to\infty}\lim_{h_t\to\infty} C_{s,t}(h_s,h_t)=0.$$

Then, because of (9), it follows that:

$$\lim_{h_s\to\infty}\lim_{h_t\to\infty} \gamma_{s,t}(h_s,h_t)=C_{s,t}(0,0).$$

Using the following relation:

$$C_{s,t}(h_s,0)=(k_1C_t(0)+k_2)C_s(h_s)+k_3C_t(0),$$

which is implicit in the product-sum covariance model, it follows that:

$$\lim_{h_s\to\infty} C_{s,t}(h_s,0)=k_3C_t(0).$$

Finally, by applying (8) it follows that:

$$\lim_{h_s\to\infty} \gamma_{s,t}(h_s,0)=C_{s,t}(0,0)-\lim_{h_s\to\infty} C_{s,t}(h_s,0)=k_sC_s(0).$$

Similarly, in order to prove (14), simply note the following:

$$C_{s,t}(0,h_t)=(k_1C_s(0)+k_3)C_t(h_t)+k_2C_s(0),$$

and (7); then it follows that:

$$\lim_{h_t\to\infty} \gamma_{s,t}(0,h_t)=C_{s,t}(0,0)-\lim_{h_t\to\infty} C_{s,t}(0,h_t)=k_tC_t(0).$$

Using (3), (4) and (5), the expression for $\gamma_{s,t}(h_s,h_t)$ can be simplified:

$$\gamma_{s,t}(h_s,h_t)=\gamma_{s,t}(h_s,0)+\gamma_{s,t}(0,h_t)-k\gamma_{s,t}(h_s,0)\gamma_{s,t}(0,h_t), \tag{15}$$

where:

$$k=\frac{k_1}{k_sk_t}. \tag{16}$$

Recalling (6), it is seen that:

$$k=\frac{k_1}{k_sk_t}=\frac{k_sC_s(0)+k_tC_t(0)-C_{s,t}(0,0)}{k_sC_s(0)k_tC_t(0)}.$$

In the process of estimating and modeling $\gamma_{s,t}(h_s,0)$ and $\gamma_{s,t}(0,h_t)$ one will have already obtained the sill values $k_sC_s(0)$ and $k_tC_t(0)$, defined in (13) and (14). Hence, in (15) k is the only remaining parameter to be estimated; note that k depends on the global sill value. The following theorem establishes a necessary and sufficient condition, given in terms of bounds on k, to ensure admissibility for $\gamma_{s,t}$ defined in (15).

Theorem 2 *Let Z be a second order stationary spatial-temporal random field. Assume that $C_{s,t}$ has the form given in (2) and that $C_{s,t}$ is continuous in space-time. Assume that for the spatial-temporal variogram defined in (15) the value of k is as defined in (16). Then $k_1 > 0, k_2 \geq 0, k_3 \geq 0$ if and only if k satisfies the following inequality:*

$$0 < k \leq \frac{1}{max\{sill(\gamma_{s,t}(h_s, 0)); sill(\gamma_{s,t}(0, h_t))\}}. \tag{17}$$

Proof. If $C_{s,t}$ is expressed as product-sum of purely spatial and temporal covariances with coefficients $k_1 > 0, k_2 \geq 0$ and $k_3 \geq 0$, and

$$k = \frac{k_1}{k_s k_t} = \frac{k_s C_s(0) + k_t C_t(0) - C_{s,t}(0,0)}{k_s C_s(0) k_t C_t(0)},$$

where $k_s C_s(0)$, $k_t C_t(0)$, $C_{s,t}(0,0)$ are the sill values of $\gamma_{s,t}(h_s, 0)$, $\gamma_{s,t}(0, h_t)$, $\gamma_{s,t}$ as in Theorem 1, it follows that:

$$k_1 = \frac{k_s C_s(0) + k_t C_t(0) - C_{s,t}(0,0)}{C_s(0) C_t(0)} > 0 \Rightarrow$$
$$\Rightarrow C_{s,t}(0,0) < k_s C_s(0) + k_t C_t(0), \tag{18}$$

$$k_2 = \frac{C_{s,t}(0,0) - k_t C_t(0)}{C_s(0)} \geq 0 \Rightarrow C_{s,t}(0,0) \geq k_t C_t(0), \tag{19}$$

$$k_3 = \frac{C_{s,t}(0,0) - k_s C_s(0)}{C_t(0)} \geq 0 \Rightarrow C_{s,t}(0,0) \geq k_s C_s(0). \tag{20}$$

By adding both sides of (19) and (20) and solving for $C_{s,t}(0,0)$, it follows that:

$$C_{s,t}(0,0) \geq \frac{k_s C_s(0) + k_t C_t(0)}{2}.$$

The last three inequalities are simultaneously satisfied when:

$$C_{s,t}(0,0) \geq max\{k_s C_s(0), k_t C_t(0)\}. \tag{21}$$

Since $k_1 > 0$ is a necessary condition for the admissibility of (2) (otherwise the model may only be semi-definite), this last condition with (4) and (5) imply that $k_s > 0$ and $k_t > 0$ (because variograms are non negative functions), then it follows that $k > 0$. Moreover, in order to satisfy (21), k must be less than or equal to $\frac{1}{max\{k_s C_s(0), k_t C_t(0)\}}$. Hence:

$$k \in \left]0; \frac{1}{max\{k_s C_s(0), k_t C_t(0)\}}\right].$$

Conversely, if k satisfies (17), then (15) will be a valid variogram. In fact, if

$$k = \frac{(sill\gamma_{s,t}(h_s, 0) + sill\gamma_{s,t}(0, h_t) - sill\gamma_{s,t}(h_s, h_t))}{(sill\gamma_{s,t}(h_s, 0)sill\gamma_{s,t}(0, h_t))},$$

(15) is equivalent to (2). The bounds on k, the inequalities in (18) and (21) imply that $k_1 > 0, k_2 \geq 0$ and $k_3 \geq 0$.

Corollary 1 *If either $\gamma_{s,t}(h_s, 0)$ or $\gamma_{s,t}(0, h_t)$ is unbounded, then there is no choice of k, satisfying the inequality (17) such that*

$$\gamma_{s,t}(h_s, h_t) = \gamma_{s,t}(h_s, 0) + \gamma_{s,t}(0, h_t) - k\gamma_{s,t}(h_s, 0)\gamma_{s,t}(0, h_t)$$

is a valid spatial-temporal variogam.

Proof. It easily follows from theorem 2.
In turn, this last result implies the following corollary.

Corollary 2 *If either $\gamma_s(h_s)$ or $\gamma_t(h_t)$ is unbounded, then (3) is not a valid model for any choice of the coefficients k_1, k_2 and k_3.*

4 A wider class of models

In Cressie and Huang (1999) the authors assume that $C_{s,t}(h_s, h_t)$ is integrable (in order to obtain a Fourier integral representation). It is easy to show that if either $k_2 \neq 0$ or $k_3 \neq 0$ then, irrespective of the choice of the models for $C_s(h_s)$ or $C_t(h_t)$, i.e., for $\gamma_s(h_s)$ or $\gamma_t(h_t)$, $C_{s,t}(h_s, h_t)$ is not integrable (in space-time). Hence, there exist models which can be obtained as (generalized) product-sum models, but cannot be derived from the integral representation proposed by Cressie and Huang (1999).
The product-sum model could be further generalized as follows:

$$\gamma_{s,t}(h_s, h_t) = (k_2 + k_1 C_t(0))\gamma_s(h_s) + (k_3 + k_1 C_s(0))\gamma_t(h_t) - k_1\gamma_s(h_s)\gamma_t(h_t) +$$
$$+ k_4\gamma 1_s(h_s) + k_5\gamma 2_t(h_t) \quad (22)$$

where γ_s and γ_t are (bounded) valid spatial and temporal variograms, $\gamma 1_s$ and $\gamma 2_t$ are valid spatial and temporal variograms (not necessarily bounded), k_4 and k_5 are non-negative constants. Adding one or more of these two terms will complicate the fitting process, however this generalization is not considered further in this paper.

5 Some practical aspects

Even though it is now possible, using either product-sums or Fourier integral representations, to generate a large class of valid spatial-temporal covariances or variograms, the problem of choosing the model and fitting it to the data, i.e., determining the parameters in the model(s), has to be faced. The fitted model can then be used to predict the spatial-temporal process at non-data locations (data location in space and non-data location in time, non-data location in space and data location in time, non-data location in space and non-data location in time).

In a strictly spatial context, structural analysis basically consists of computing the sample variogram and fitting a valid model to it. Although there may be complications due to anisotropies or non-stationarity, the procedure will still involve these steps. The process is practical, since a large class of known valid models is available and additional models can be generated as positive convex combinations of the simpler models. Moreover, there are three basic geometric features to look for in plotting the sample variogram that can be used to choose the type of model. Anisotropic models are variations of isotropic models. This procedure does not work so well in the space-time context. The problem of valid models, which has been discussed above, and the problem of fitting the data to a model, have to be addressed. In De Cesare, et al. (1997) and in De Cesare et al. (2001), spatial and temporal variograms were separately estimated and modeled from data. These models were then combined, as in the product model or in the product-sum model, to obtain the final spatial-temporal model. This reduced the problem to essentially the same techniques used in the strictly spatial context. Least squares could also be used as scheme to determine the parameters in either or both of the variogram components. Note that using least squares still requires determining the model type(s) separately. For a diagnostic check of their results, Cressie and Huang (1999) simply picked three different models obtained from the Fourier integral representation and then used least squares to determine the parameters in the models. The model with the smallest weighted least squares was selected. However this technique does not ascertain whether there might be another model that would result in a smaller weighted least squares. Apart from the added unbounded variogram component, their models are necessarily integrable, hence the class of models is limited in that respect.

As shown above, the general product-sum model defined in (15), depends solely on the parameter k, hence on the global sill $C_{s,t}(0,0)$ (assuming that the separate spatial and temporal variograms have been fitted). The problem of computing the parameter k is now addressed.
Given the set of data locations in space-time

$$A = ((s_i, t_j), i = 1, 2 \ldots, n_s, j = 1, 2, \ldots, n_t),$$

estimating and modeling the spatial and temporal components proceeds as follows:

1. Compute the sample spatial and temporal variograms corresponding to $\gamma_{s,t}(h_s, 0)$ and $\gamma_{s,t}(0, h_t)$,

$$\widehat{\gamma}_{s,t}(r_s, 0) = \frac{1}{2|N(r_s)|} \sum_{N(r_s)} [Z(s + h_s, t) - Z(s, t)]^2, \tag{23}$$

$$\widehat{\gamma}_{s,t}(0, r_t) = \frac{1}{2|M(r_t)|} \sum_{M(r_t)} [Z(s, t + h_t) - Z(s, t)]^2, \tag{24}$$

   where r_s and r_t are, respectively, the vector lag with spatial tolerance δ_s and the lag with temporal tolerance δ_t. $|N(r_s)|$ and $|M(r_t)|$ are the cardinalities of the following sets:

$$N(r_s) = \{(s + h_s, t) \in A, (s, t) \in A : ||r_s - h_s|| < \delta_s\},$$
$$M(r_t) = \{(s, t + h_t) \in A, (s, t) \in A : ||r_t - h_t|| < \delta_t\};$$

2. Choose valid variogram models $\gamma_{s,t}(h_s, 0)$ and $\gamma_{s,t}(0, h_t)$ for the above two variogram estimators. Note that at this point, one must use models with sills. Hence estimates for the sill values $k_s C_s(0)$ and $k_t C_t(0)$ are obtained;

3. Compute the sample variogram corresponding to $\gamma_{s,t}(h_s, h_t)$, namely:

$$\widehat{\gamma}_{s,t}(r_s, r_t) = \frac{1}{2|L(r_s, r_t)|} \sum_{L(r_s,r_t)} [Z(s + h_s, t + h_t) - Z(s, t)]^2, \tag{25}$$

   where $|L(r_s, r_t)|$ is the cardinality of the set $L(r_s, r_t)$, that is:

$$\{(s + h_s, t + h_t) \in A, (s, t) \in A : ||r_s - h_s|| < \delta_s \text{ and } ||r_t - h_t|| < \delta_t\};$$

4. Estimate the global sill $C_{s,t}(0, 0)$. There are two alternative methods:

   - graphically, by plotting the sample variogram surface $\widehat{\gamma}_{s,t}(r_s, r_t)$;
   - fitting $\widehat{\gamma}_{s,t}(r_s, r_t)$ to the space-time variogram (15). In this last case $C_{s,t}(0, 0)$ can be estimated by minimizing $W(C_{s,t}(0, 0))$, the weighted least-squares value (Cressie, 1993), given by:

$$W(C_{s,t}(0, 0)) =$$
$$= \sum_{s}^{L_s} \sum_{t}^{L_t} |L(r_s, r_t)| \left(\frac{\widehat{\gamma}_{s,t}(r_s, r_t) - \gamma_{s,t}(h_s, h_t; C_{s,t}(0, 0))}{\gamma_{s,t}(h_s, h_t; C_{s,t}(0, 0))} \right)^2,$$

where L_s and L_t are, respectively, the number of spatial vector lags and the number of temporal lags. Once a spatial-temporal model has been fitted, cross-validation provides an additional diagnostic for judging the fit.

5. Once the three sills have been estimated, the value of k parameter is determined, of course one must check that (17) is satisfied.

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