Estimating and Modeling Space-Time Variograms

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Abstract

As with a spatial variogram or spatial covariance, a principal purpose of estimating and modeling a space-time variogram is to quantify the spatial temporal dependence reflected in a data set. The resulting model might then be used for spatial interpolation and/or temporal prediction which might take several forms, e.g. kriging and Radial Basis functions. There are significant problems to overcome in both the estimation and the modeling stages for space-time problems unlike the purely spatial application where estimation is the more difficult step. The key point is that a spatial-temporal variogram as a function must be conditionally negative definite (not just semi-definite) which can be a difficult condition to verify in specific cases. In the purely spatial context one relies on a known list of isotropic valid models, e.g., the Matern class as well as the exponential and gaussian models, as well as on positive linear combinations of known valid models. Bochner's Theorem (or the extension given for generalized covariances by Matheron) characterizes non-negative definite functions but does not easily distinguish the strictly positive definite 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 for space-time is to "separate" the dependence on space and on time. This is not new and in fact a similar problem can occur in spatial application, i.e., a zonal anisotropy. Early attempts used either the sum of two covariances or the sum of two variograms, in either case one component being defined on space and the other on time. It is easily shown that this leads to semi-definite models and hence if used in kriging equations, the result may be a non-invertible coefficient matrix. It is also easy to see that the product of two variograms (even on the same domain) can violate the growth condition. However it is well known that the product of two strictly positive definite functions is again strictly positive definite. In fact a gaussian covaiance model might be viewed as product (of several gaussian models each defined on a lower dimensional space). Likewise one form of the exponential covariance, often used in hydrology applications, is also a product. When converted to variogram form, there is not only a product (with a negative sign) but also a sum. It turns out that the variogram form is more convenient in the estimation stage.

The simple product covariance is somewhat too limiting however, each component effectively must have the same "sill". An obvious extension is the product-sum model which when converted to variogram form is the same as for the product (but with different coefficients), This can be further generalized to an integrated product sum model.

In the estimation stage there are two separate problems, one is to determine the appropriate model type and the other is to estimate the model parameters. In a typical spatial application the list of possible models is usually kept small and hence the primary emphasis is on estimating the model parameters. In the spatial

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temporal context the list of possible models is likely to be much greater and model type selection more difficult. De Ioca, Myers and Posa have shown that the use of marginal variograms is one way to attack this problem and have given an example of extending to the integrated product sum model as well as to the multivariate case using a Linear Coregionalization Model.

1.Introduction

Interpolation in a purely spatial context using geostatistical techniques usually involves two steps: (1) estimating or modeling the mean function, (2) estimating and modeling the spatial structure function, i.e., the covariance function or variogram. Of course these two are connected since the data is not *a priori* split into data for the mean and data for the structure function. The second step typically involves invoking a form of stationarity, second order or intrinsic. Interpolation and prediction for space-time data is similar but more complicated for several reasons. Kyriakidis and Journel (1999) have given an extensive review of both the various models and the problems arising in step (1) for spatial-temporal data. Although a non-trivial aspect of the problem, the following focuses on the second step, i.e., estimating and modeling the structure function. Both the kriging estimator and the kriging equations are essentially dimension free, in particular they have the same form for spatial-temporal problems as for purely spatial problems. One critical problem arises however, a covariance function must be strictly positive definite and a variogram must be strictly conditionally negative definite to ensure that the kriging equations have a unique solution. In the spatial context, this problem is easily resolved by choosing the covariance function or variogram from a list of functions known to satisfy the appropriate definiteness condition. "Choosing" is the operative word because for most applications it is not possible to derive the appropriate structure function from first principles. The "list" is actually for isotropic models, geometric anisotropies being incorporated by allowing the range of the model to change with direction. Time might be considered as simply another dimension but this imposes severe restrictions. Until very recently however a comparable list of valid spatial-temporal covariance functions or variograms was not available. The product-sum model and its extensions as given in De Iaco , Myers and Posa (2002a) is a step in that direction.

2. The Random Function

Let $Z(\mathbf{s},t)$ denote a real valued random function defined on $R^d \times T$. For simplicity as indicated above it is assumed that $E[Z(\mathbf{s},t)]$ exists and is constant. In a typical application, $d = 2$ or 3 but none of the following results depend on that assumption. Assuming that $Z(\mathbf{s},t)$ is second-order stationary then the covariance function is given by

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

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

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

As is well known under the stronger assumption

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

Although in much of what follows the stronger assumption of second order stationarity will be used, it will generally be convenient to express the results in terms of variograms. Two additional functions are useful, called the "marginals" by analogy with marginals for probability density or probability distribution functions. $C_{ST}(\mathbf{h}_s,0)$, $C_{ST}(\mathbf{0}, h_t)$ respectively are the spatial and temporal marginal covariances. Likewise $\gamma_{ST}(\mathbf{h}_s, 0)$, $\gamma_{ST}(\mathbf{0}, h_t)$ are the spatial and temporal marginal variograms.

3. Practical Questions

As noted above, it is important for a space-time covariance function to be strictly positive definite (not just non-negative definite) and likewise for a space-time variogram to be strictly conditionally negative definite (not just non-positive definite). Thus only models satisfying this restriction will be of interest. Given a spatial-temporal data set it is important to be able to "fit" a model to the data, a covariance function or a variogram. While it is common and often easy to collect data at regular time points, regularity in space is not so common. Moreover if data is collected by some form of automatic equipment, e.g., air quality monitoring, the number of distinct time points may be quite large whereas the number of spatial data locations relatively small. This in turn can create difficulties in fitting a structure function. Even if some form of least squares is used to fit the covariance function or the variogram it is still necessary to choose a model type or types. Thus both a list of valid models is needed and also a scheme for choosing from the list.

4. Basic Models

4.1 Sum

The two simplest ways for constructing a spatial-temporal model are (1) treat space and time completely separately, (2) treat time as simply another dimension, albeit perhaps with a different unit of measurement. The latter essentially implies the use of a metric or distance function on space-time. The former corresponds to what has sometimes been called a "zonal" anisotropy. The zonal or “sum” model is of the form

$$C_{ST}(\mathbf{h}_s, h_t) = C_S(\mathbf{h}_s) + C_T(h_t) \quad (1)$$

or

$$\gamma_{ST}(\mathbf{h}_s, h_t) = \gamma_S(\mathbf{h}_s) + \gamma_T(h_t) \quad (2)$$

where $C_S(\mathbf{h}_s)$ and $C_T(h_t)$ are spatial and temporal covariances respectively, $\gamma_S(\mathbf{h}_s)$ and $\gamma_T(h_t)$ are spatial and temporal variograms respectively. Unfortunately even if these separate spatial and temporal covariances satisfy the strict definiteness conditions, and the separate spatial and temporal variograms satisfy the strict condtional negative definiteness condition, the resulting spatial-temporal covariance function and spatial-temporal variogram do not. This was as shown by a simple example in Myers and Journel (1990). Also see Rouhani and Myers (1990), Dimitrakopoulos and Luo(1994). However the sum construction is nearly an acceptable model, i.e., it only fails the strict definiteness condition. Hence a reasonable question to ask might be, is there a function G(u,v) on R^2 such that

$$\gamma_S(\mathbf{h}_s) + \gamma_T(h_t) + G(\gamma_S(\mathbf{h}_s), \gamma_T(h_t)) \quad (3)$$

is a strictly conditionally negative definite function. As will be seen later there is at least one such function.

4.2 Metric

Let $C(\mathbf{u})$ is a strictly positive definite function on R^{d+1} and $\gamma(\mathbf{u})$ is strictly conditionally negative definite on R^{d+1} . If $R^d \times T$ is simply considered as a d+1 dimensional space then

$$C_{ST}(\mathbf{h}_s, h_t) = C(|\mathbf{h}_s| + a|h_t|) \quad (4)$$

and

$$\gamma_{ST}(\mathbf{h}_s, h_t) = \gamma(|\mathbf{h}_s| + a|h_t|) \quad (5)$$

are valid models on $R^d \times T$, a >0. This model has been used by several authors. Its properties will be discussed later.

4.3.1 Alternative Metric

As noted by Dimitrakopoulos and Luo(1994) instead of using $|\mathbf{h}_s| + a|h_t|)$ as a distance function on $R^d \times T$,one might use $|\mathbf{h}_s|^2 + a|h_t|^2)$. In terms of the topology, these two are equivalent.

4.4 Sum-Metric

One way to resolve the problem with the zonal model is to combine it with a metric model, i.e.,

$$\gamma_{ST}(\mathbf{h}_s, h_t) = \gamma_S(\mathbf{h}_s) + \gamma_T(h_t) + \gamma(|\mathbf{h}_s| + a|h_t|) \tag{6}$$

or

$$\gamma_{ST}(\mathbf{h}_s, h_t) = \gamma_S(\mathbf{h}_s) + \gamma_T(h_t) + \gamma(|\mathbf{h}_s|^2 + a|h_t|^2) \tag{7}$$

4.5 Product

Let $Z_1(\mathbf{s})$ and $Z_2(t)$ be uncorrelated random functions defined on R^d ,T respectively with strictly positive definite covariance functions $C_S(\mathbf{h}_s)$, $C_T(h_t)$ Then the covariance function of $Z(\mathbf{s},t) = Z_1(\mathbf{s})\, Z_2(t)$ is

$$C_{ST}(\mathbf{h}_s, h_t) = C_S(\mathbf{h}_s) \times C_T(h_t) \tag{8}$$

If both factors are strictly positive definite then $C_{ST}(\mathbf{h}_s, h_t)$ is strictly positive definite on $R^d \times T$. In variogram form this becomes

$$\gamma_{ST}(\mathbf{h}_s, h_t) = C_T(0)\gamma_S(\mathbf{h}_s) + C_S(\mathbf{0})\gamma_T(h_t) - \gamma_S(\mathbf{h}_s) \times \gamma_T(h_t) \tag{9}$$

or in terms of the marginals

$$\gamma_{ST}(\mathbf{h}_s, h_t) = \gamma_{ST}(\mathbf{h}_s, 0) + \gamma_{ST}(\mathbf{0}_s, h_t) - [1/C_T(0)C_S(\mathbf{0})]\gamma_{ST}(\mathbf{h}_s, 0)\times \gamma_{ST}(\mathbf{0}_s, h_t) \tag{10}$$

For examples of the use of the product covariance see De Cesare , Myers and Posa (1997) as well as others.

5. The Product-Sum

It is seen then that the "sum" and the "product" are basic combinations that might be used to generate spatial-temporal variograms. Each separately has disadvantages or limitations which the combination does not have. As introduced in De Cesare, Myers and Posa (2001a), De Cesare, Myers and Posa (2001b), De Iaco, Myers and Posa (2001), De Iaco, Myers and Posa (2002a) the product-sum covariance is given by

$$C_{ST}(\mathbf{h}_s, h_t) = k_1 C_S(\mathbf{h}_s) \times C_T(h_t) + k_2 C_S(\mathbf{h}_s) + k_3 C_T(h_t) \tag{11}$$

with $k_1 > 0$, $k_2 \geq 0$, $k_3 \geq 0$. Again if $C_S(\mathbf{h}_s)$ and $C_T(h_t)$ are strictly positive definite then $C_{ST}(\mathbf{h}_s, h_t)$ is strictly positive definite on $R^d \times T$. The variogram form is somewhat more convenient

$$\gamma_{ST}(\mathbf{h}_s, h_t) = [k_1 C_T(0) + k_2]\gamma_S(\mathbf{h}_s) + [k_1 C_S(\mathbf{0}) + k_3]\gamma_T(h_t) - k_1\gamma_S(\mathbf{h}_s) \times \gamma_T(h_t) \tag{12}$$

or

$$\gamma_{ST}(\mathbf{h}_s, h_t) = \gamma_{ST}(\mathbf{h}_s, 0) + \gamma_{ST}(\mathbf{0}_s, h_t) - K\gamma_{ST}(\mathbf{h}_s, 0)\times \gamma_{ST}(\mathbf{0}_s, h_t) \tag{13}$$

As was shown in De Iaco, Myers and Posa (2001) the necessary and sufficient condition for K is

$$0 < K \leq 1/\max(\text{sill } \gamma_{ST}(\mathbf{h}_s, 0) , \text{sill } \gamma_{ST}(\mathbf{0}_s, h_t)) \tag{14}$$

Application examples are found in De Iaco, Myers and Posa (2000, 2002b)

5.1 Two Special Products

5.1.1 Exponential

In Eq (4) let C(u) = Exp(-u) then the metric model becomes

$$C_{ST}(\mathbf{h}_s, h_t) = \quad Exp(-|\mathbf{h}_s| - a|h_t|) = Exp(-|\mathbf{h}_s|)Exp(-a|h_t|) = \quad C_S(\mathbf{h}_s) \times C_T(h_t) \qquad (15)$$

That is, the metric model is actually the product of two exponential models. The product-sum then provides a generalization of the metric model

$$\gamma_{ST}(\mathbf{h}_s, h_t) = A[1- Exp(-|\mathbf{h}_s|)] + B[1- Exp(-a|h_t|)] - KAB [1- Exp(-|\mathbf{h}_s|)][1- Exp(-a|h_t|)] \qquad (16)$$

If $A = B$ and $K = 1/A$ then the model is again just the exponential model, i.e., the metric model.

5.1.2 Gaussian

Using the alternative metric as in Section 4.3.1 and again with $C(u) = Exp(-u)$ we obtain

$$C_{ST}(\mathbf{h}_s, h_t) = \quad Exp(-|\mathbf{h}_s|^2 - a|h_t|^2) = Exp(-|\mathbf{h}_s|^2)Exp(-a|h_t|^2) = \quad C_S(\mathbf{h}_s) \times C_T(h_t) \qquad (17)$$

Again the metric model is actually a product, this time the product of two gaussian models. In variogram form this becomes

$$\gamma_{ST}(\mathbf{h}_s, h_t) = A[1- Exp(-|\mathbf{h}_s|_2)] + B[1- Exp(-a|h_t|^2)] - KAB [1- Exp(-|\mathbf{h}_s|^2)][1- Exp(-a|h_t|^2)] \qquad (18)$$

6.Integrated Product-Sum

Let $f(u)$ be a probability density function on R^k and $\gamma_{ST}(\mathbf{h}_s, h_t ; \alpha)$ be a strictly conditionally negative definite function on $R^d \times T$ for each α in the support of $f(u)$. Then

$$\int \gamma_{ST}(\mathbf{h}_s, h_t ; \alpha) f(\alpha) d\alpha \qquad (19)$$

is likewise a strictly conditionally negative definite function on $R^d \times T$. Examples for various choices of product-sum variograms and various probability density functions are found in De Iaco, Myers and Posa (2002a). The result could equally well be given in terms of covariance functions and obviously also in terms of the corresponding correlation functions. The construction given by Cressie and Huang (1999) is similar but stated in terms of covariance functions.

6.1 Mixture Models

Ma (2002) has proposed the following mixture model, given terms of correlation functions. Let $\rho_S(\mathbf{h}_s) \times \rho_T(h_t)$ be the correlation functions corresponding to the covariance functions in Eq (8). The proposed positive mixture model is

$$\rho_{ST}(\mathbf{h}_s, h_t) \quad = \sum_{[i=0,\dots]} \sum_{[j=0,\dots]} [\rho_S(\mathbf{h}_s)]^i \times [\rho_T(h_t)]^j \, p_{ij} \qquad (20)$$

where p_{ij} is a bivariate probability density on the positive integers. For notational convenience assume $0^0 = 1$. Ma gives a number of examples using various choices of the probability density. Note that this can be considered a special case of Eq (19) by the following substitutions

$$[\rho_S(\mathbf{h}_s)]^i \quad = \quad [1- \gamma_S(\mathbf{h}_s)/C_S(\mathbf{0})]^i , \quad [\rho_T(h_t)]^j = \quad [1-\gamma_T(h_t)/C_T(0)]^j \qquad (21)$$

Alternatively, simply consider $\rho_{ST}(\mathbf{h}_s, h_t;(i,j)) = [\rho_S(\mathbf{h}_s)]^i \times [\rho_T(h_t)]^j = [1- \gamma_{ST}(\mathbf{h}_s, h_t;(i,j))/[C_S(\mathbf{h}_s)]^i [C_T(h_t)]^j]$. Since each $\rho_S(\mathbf{h}_s)$ and $\rho_T(h_t)$ are assumed strictly positive definite, $\rho_{ST}(\mathbf{h}_s, h_t;(i,j))$ will be strictly conditionally positive definite for each pair $(i,j) = \alpha$. Hence the corresponding variogram $\gamma_{ST}(\mathbf{h}_s, h_t;(i,j))$ will be strictly conditionally negative definite for each pair (i.j). In this case the integral in Eq (19) reduces to a double summation.

7. Model Properties

7.1 Sum Model

Let $\gamma_{ST}(\mathbf{h}_s, h_t)$ be a sum-zonal model as in Eq (2). The spatial and temporal marginals are $\gamma_S(\mathbf{h}_s)$, $\gamma_T(h_t)$ respectively. Either component can be unbounded, e.g. a power model. If either component is unbounded then $\gamma_{ST}(\mathbf{h}_s, h_t)$ is unbounded. Because this is a separable model, a geometric anisotropy could be incorporated into the spatial component. The continuing difficulty however is that the coefficient matrix in the kriging system will in general be non-invertible. Some authors have suggested that because the coefficient matrix may be invertible for some data location patterns it would satisfactory to use such a model as for example in Buxton and Pate (1994). However the change from invertibility to non-invertibility will not be a jump discontinutiy and hence the results will always be suspect.

7.2 Metric Model(s)

Irrespective of which form of the metric is used, a pure metric model is rather restricted. Both marginals will be of the same type and have the same sill (if the model is bounded), only the range parameter changes. Hence it is much more likely that a sum-metric model would be chosen, i.e., as in Eq (6) or Eq (7). The respective marginals then are

$$\gamma_{ST}(\mathbf{h}_s, 0) = \gamma_S(\mathbf{h}_s) + \gamma(|\mathbf{h}_s|), \quad \gamma_{ST}(0, h_t) = \gamma_T(h_t) + \gamma(a|h_t|) \tag{22}$$

The strict conditional negative definiteness is ensured by that property for γ hence the other two components could in fact be only semi-definite. If any of the three components is unbounded then $\gamma_{ST}(h_s, h_t)$ is unbounded. Since there are three different model types to be determined (along with their parameters) this model will be more difficult to fit to data.

7.3 Product and Product-Sum Models

Since the Product model can be considered a special case of the product sum model most of its properties can be deduced from those of the Product-Sum. However the Product-Sum has an extra parameter and hence is much more general, i..e, for a given pair of variograms there is an entire class of spatial-temporal variograms. One for each choice of K. It is easy to see the marginals for the Product-Sum model from Eq (13). Moreover the marginals can be directly estimated from data. Unlike the sum, metric and sum-metric the second order stationarity assumption is essential here.

7.4 Integrated Models

It is easy to see that the marginals of the integrated model in Eq (19) are

$$\int \gamma_{ST}(\mathbf{h}_s, 0; \alpha) f(\alpha) d\alpha \,, \qquad \int \gamma_{ST}(\mathbf{0}, h_t ; \alpha) f(\alpha) d\alpha \tag{23}$$

7.5 Unbounded Components

There are actually two additional marginals, namely $\gamma_{ST}(h_s, \infty)$ and $\gamma_{ST}(\infty, h_t)$. These are not likely of any interest in the case of the sum or sum-metric models. In either the Product or Product-Sum models however these provide some information. Under the second order stationarity assumption for both the spatial and temporal components both of these additional marginals are bounded, e.g., a Product or Product-Sum model. However it is easy to see that more generally they need not be. The evidence for such behavior would be reflected in the sample variogram and the sample marginal variograms. As noted by Cressie and Huang (1999) it is always possible to add an unbounded component, either spatial or temporal.

7.6 Product-Sum models and the LCM

As shown in De Iaco, Myers and Posa (2003) it is easy to incorporate the Product-Sum model into a Linear Coregionalization Model (LCM). Each component in the LCM can be written as a Product-Sum, this gives rise to an extended form of the marginals and some limitations in fitting the data.

8. Fitting Data to the Model

As in the purely spatial context, there are usually two separate stages: (1) choosing the model (or the components of the model),(2) estimating the parameters of the model. In both stages the simplest approach to fitting space-time data to a spatial-temporal covariance function or variogram is to reduce the problem to one similar to those encountered in a purely spatial context. Since there is no universal model some form of sample covariance or sample variogram is usually necessary. The problem then is how to interpret the results. One solution is the use of marginals to determine the model types. After that step it would still be possible to determine the parameters using weighted least squares. Cross validation, Myers (1991) can be used to evaluate the resulting fit.

8.1 Using Marginals

Under the second order stationarity assumption the marginal variograms can be estimated by (1) computing the sample spatial variograms for each data time point and then averaging over time, (2) computing the sample temporal variograms for each data spatial location and then averaging over space. De Cesare, Myers and Posa (2000) have given a modification of the GSLIB sample variogram code for these purposes. Example applications are found in De Cesare, Myers and Posa (1997), De Iaco, Myers and Posa (2000), De Iaco, Myers and Posa (2003).

9. References

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