On smoothness measures for space-time surfaces

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Abstract The differentiability of a stochastic process has a direct relationship with the differentiability of covariance function. Space-time geostatistics have had recently a great development, and new families of covariance functions have been proposed following different methodologies. However, although they are positive definite, not all of them represent the reality of a particular phenomenon of study. Therefore, the analysis of other properties is necessary before choosing the suitable model. Here we presented a review of the concept of differentiability of both, space–time covariance models and stochastic process, and its implications on correlations of linear combinations underlying observations, specifically, in the increments. We analyze the change of the function of covariance from the origin and as lag grows. The predictions depend on the values that the covariance function takes. So, by using the concept of smoothness of a covariance function, which can be considered as the geometrical view of the differentiability, we determine some characteristics of the predictions obtained with these covariance functions. We propose two ways of measuring the smoothness of any covariance function. For illustrative purposes, we apply them to purely spatial covariance functions and to several space-time covariance models, and we show a characterization of these models according to their smoothness.
1 Introduction

[3] shows that these covariance functions that are not smoother away from the origin than at the origin, generate discontinuities in some correlations of linear combinations of the stochastic process \( Z \), specifically in the correlations between increments. Proposition 1 shows a characterization of certain types of covariance models. However, several covariance models are analytic and do not accomplish with the hypothesis of this proposition. It is then, necessary to find a way to measure smoothness, available for any covariance model. As known it is, the kriging predictor is a linear combination of the observations. The increments have a special interest because, we can observe the change of the covariance function when a lag grows from the origin and how this behavior affects the predictions. We use a concept of smoothness, which can be considered as a geometric vision of the differentiability. We thus propose to measure the smoothness of surfaces generated by covariance functions to analyze the continuity of the associated process, which will have a direct impact on predictions.

We now present the definitions of the derivatives of a stochastic process, and the theorem that shows the relation between them and its covariance function, [8], which are the basic elements for Proposition 1.

**Definition 1 (Derivate of a stochastic process).**

Let \( Z(x) \in \mathbb{R}^n \) be a stochastic process with covariance function depending on the index set \( C(x,y) \); the associated gradient \( \dot{Z}(x) \) is a vector in the space \( \mathbb{R}^n \) defined in a Cartesian coordinate system by its components:

\[
\dot{Z}_i(x) = \frac{\partial Z(x)}{\partial x_i} = \lim_{h \to 0} \frac{Z(x + he_i) - Z(x)}{h}
\]

(1)

where \( e_i \) is a unitary vector in the \( i \)-th direction and \( h \) is a scalar; \( i = 1, ..., n \).

*The general derivate of order \( m \) of the process \( Y \), is*

\[
Z^m(x) = \frac{\partial |m| Z(x)}{\partial x_1^{m_1} ... \partial x_n^{m_n}}
\]

(2)

where \( |m| = \sum_{i=1}^n m_i \).

**Theorem 1.** Let \( Z(x) \in \mathbb{R}^n \) be a stochastic process with covariance function \( C \) and expectation \( E(Z) \) differentiables. If

\[
\frac{\partial^2}{\partial x_i \partial y_j} C(x,y)
\]

exists and is finite for all \( i = 1, ..., n \) at the point \( (x,x) \), then \( Z(x) \) is mean-square differentiable in \( x \), and (3) is the covariance function of the process \( \dot{Z}_i(x) \).

Thus, for a stationary random field, the behavior of its covariance function in the neighborhood of the origin, allows to determine its second order properties. This concept can be generalized to derivatives of any order \( m \). If the derivate
\[
\frac{\partial^{2|m} C(x, y)}{\partial x_1^{m_1} \cdots \partial x_n^{m_n} \partial y_1^{n_1} \cdots \partial y_n^{n_n}} (4)
\]
exists and is finite for all \( i = 1, \ldots, n \) at the point \((x, x)\), the process \(Z(x)\) is mean-square differentiable in \(x\), and (4) is the covariance function of the process \(Z^m(x)\).

For \(m \geq 0\), and if \(Z(x, y)\) is \(m\) times mean-square differentiable in its first coordinate, and we write \(Z^m(x, y)\), for this \(m\)-th mean-squared derivative, [3] defines the autocorrelation of the increments for small lags as:

\[
\rho^m_\varepsilon (x, y) = \text{corr}(Z^m(\varepsilon, 0) - Z^m(0, 0), Z^m(x + \varepsilon, y) - Z^m(x, y)) (5)
\]

and let \(\rho^m\) be its limit when \(\varepsilon \to 0\).

**Proposition 1 (Stein, 2005).** [3]

Suppose that \(C^m\) is a continuous function on \(\mathbb{R}^2\), \(0 < \alpha_1 < \ldots < \alpha_p < 2\), \(C_1, C_2, \ldots, C_p\) are even functions on \(\mathbb{R}\), with \(C_1(0) \neq 0\), such that

\[
C^m(x, y) = C^m(0, y) + \sum_{j=1}^p C_j(y) |x|^{\alpha_j} + R_y(x) (6)
\]

where, for any given \(y\), \(R_y(x) = O(x^2)\) as \(x \to 0\), and \(R_y(\cdot)\) has a bounded second derivative. Then

\[
\sup_{x \in \mathbb{R}} \lim_{\varepsilon \to 0} \left| \frac{C_1(y) \{ |x + \varepsilon|^{\alpha_1} - 2|x|^{\alpha_1} + |x - \varepsilon|^{\alpha_1} \}}{2C_1(0)\varepsilon^{\alpha_1}} - \rho^m_\varepsilon (x, y) \right| = 0
\]

and \(\rho^m(x, y)\) exists for all \((x, y)\) with

\[
\rho^m(x, y) = \begin{cases} 
C_1(y) & \text{if } x = 0 \\
C_1(0) & \text{if } x \neq 0 
\end{cases}
\]

Under the hypothesis of stationarity, all covariance functions are smooth away from the origin. Then, the important issue is to determine if the function presents the same behavior near the origin, at neighborhoods of 0. Besides, it is important to look for ridges, that is for local extrema.

### 2 Space-time processes

A Space-time process is a stochastic process \(\{Y(s, t) : (s, t) \in D_s \times D_t\}\), where \(D_s \times D_t\) is the space-time index set. \(D_s \times D_t \subseteq \mathbb{R}^d \times \mathbb{R}\) with \(\mathbb{R}^d\) for the space and \(\mathbb{R}\) for the time. When \(D_s\) is continuous, the process is called a geostatistical process. This approach fits models based on a finite number of Space-time observations. A general form of expressing the space-time observations of the phenomenon of interest is, [6],
\[ Y \equiv (Y(s_i; t_{ij}) \quad i = 1, \ldots, m \quad j = 1, \ldots, T) \quad (7) \]

- \( \{s_1, \ldots, s_m\} \) are the \( m \) known spatial locations,
- \( T \) is the length of the time series available at each of the \( m \) locations.

In this work, we assume that the covariance function is stationary in space and time. That is, given that \( \text{Var}(Y(s; t)) < \infty, \forall s \in D_s \) and \( \forall t \in D_t \), the mean is constant and the covariance function \( C \), only depends on the space-time lag, \( (s_i - s_{i'}, t_{ij} - t_{ij'}) \):

\[ E(Y(s, t)) = \mu \quad \text{and} \quad \text{Cov}(Y(s_i, t_{ij}), Y(s_{i'}, t'_{ij})) = C(h, u) \quad (8) \]

where \( h = s_i - s_{i'}, \quad u = t_{ij} - t'_{ij} \). Although the covariance function must be nonnegative definite, we only consider the positive definite case. That is, for any finite number \( m \) of space-time locations \( (s_1, t_1), (s_2, t_2), \ldots, (s_m, t_m) \) and any set of complex numbers, \( \{a_1, a_2, \ldots, a_m\} \) with \( m \in \mathbb{Z}^+ \), \( C \) is such that

\[ \sum_{k=1}^{m} \sum_{k'=1}^{m} a_k \overline{a_{k'}} C(s_k - s_{k'}; t_k - t_{k'}) > 0 \quad (9) \]

To ensure positive definiteness of \( C(\cdot, \cdot) \), we often use models which belong to a parametric family \( C^0 \), where all members satisfy (9).

\[ \text{Cov}(Y(s_i, t_{ij}), Y(s_{i'}, t'_{ij})) = C^0(s_i - s_{i'}; t_{ij} - t'_{ij}\mid \theta) \]  

where \( C^0 \) is a positive definite function for each parameter vector \( \theta \in \Theta \subset \mathbb{R}^p \).

A tool commonly used to reduce the number of parameters is to use a separable structure. In a space-time process, separability means that the modeling of space and time covariance, can be made individually. That is, the space-time covariance matrix \( \Sigma_{Y}^{st} \) can be the Kronecker product between the purely spatial covariance matrix, and the purely temporal covariance matrix \( \Sigma^{s} \otimes \Sigma^{t} \). \( C_{st}(h, u) = C_s(h)C_t(u) \). This method avoids the difficulties with the calculus of the inverse space-time covariance matrix.

Although this approach is computationally simpler, does not take into account the space-time interaction. In most of the cases, it exists that interaction; the effect of a change in the spatial location is different for each time; that is, the spatial dependence model varies with time. Models taking into account this interaction are called nonseparable. There are several options of parametric families: [1] built stationary nonseparable space-time covariance functions by finding the inverse Fourier transform of spectral densities. Specifically, [1] considered functions of the form

\[ C(h, u) = \int \exp(ih'\omega) \rho(\omega, u)d\omega \quad (h, u) \in \mathbb{R}^d \times \mathbb{R} \quad (11) \]
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where $\rho(\omega, u)$, $u \in \mathbb{R}$, is a continuous positive definite function for all $\omega \in \mathbb{R}^d$. However, nonseparable models could emerge as special cases. Therefore, this method requires Fourier transform pairs having a closed form.

[2] proposed a family of space-time covariance functions which unlike the former does not depend on the existence of Fourier Transform. This method is given by theorem 2.

**Theorem 2 (Gneiting’s theorem).** Let $\phi(r)$, $r \geq 0$, be a completely monotone function, and let $\phi(r)$, $r \geq 0$, be a positive function with a completely monotone derivate. Then

$$C(h, u) = \frac{\sigma^2}{\phi(u^2)} \phi \left( \frac{\|h\|^2}{\phi(u^2)} \right), \quad (h, u) \in \mathbb{R}^d \times \mathbb{R}$$

is a space-time covariance function.

There are several other methodologies to build nonseparable space-time covariance functions. To mention some, [4] proposed a product-sum model,

$$C_s(t; h, u) = aC_s(h, \theta)C_t(u, \theta) + bC_h(h, \theta) + cC_t(u, \theta)$$  \hfill (13)

where $a, b, c$ are nonnegative coefficients and $C_s(h, \theta)$ and $C_t(u, \theta)$ are covariance functions in the space and time, respectively.

[5] presented another method by using the integration of the product between $C_s(h, \theta)$ and $C_t(u, \theta)$ with respect to measure $\mu$ over the space of the parameters $\Theta$.

[7] obtain a valid model with the convex sum:

$$C_{(s,t)}(h, u) = \vartheta \phi(||h||) + (1 - \vartheta) \phi(|u|)$$

\hfill (14)

where $\vartheta \in [0, 1]$. This model is valid given that $\theta < \frac{7 - \epsilon}{1 + \epsilon}$ and $\epsilon < 7$.

Besides, [3] presented a method to build nonstationary models by using the Matern covariance function. Nevertheless, in general, the closed expressions for the covariance function rarely are found using this method.

### 3 Fundamental forms and curvatures

We now present some concepts of differential geometry, which are basic for the definitions of smoothness measures.

The first fundamental form allows to measure lengths of curves, angles between two curves in a point on the surface and areas of regions. Let $\mathcal{S}(w, v)$ be a parametrized surface and $\mathcal{S}(w(l), v(l))$ be a regular curve over it, with arc length $s$, given by the next integral

$$s(l) = \int_{l_0}^{l} \sqrt{\mathcal{S}'(\xi)^2} d\xi$$

\hfill (15)
where

\[ S'(l) = S_w \frac{dw}{dl} + S_v \frac{dv}{dl} \]  

(16)

The first fundamental form \( I \) is always positive, because it is the square of the arc length (15):

\[ I = \left( \frac{ds}{dl} \right)^2 = E \left( \frac{dw}{dl} \right)^2 + 2F \frac{dw}{dl} \frac{dv}{dl} + G \left( \frac{dv}{dl} \right)^2 \]  

(17)

where

\[ E = S_w \cdot S_w; \quad F = S_w \cdot S_v; \quad G = S_v \cdot S_v \]  

(18)

Besides, \( EG - F^2 > 0 \) because

\[ \| S_w \times S_v \| = EG - F^2 \]  

(19)

The second fundamental form provides information about the deviation of the surface from its tangent plane in the neighborhood of the point of tangency, [9]. The unitary normal vector to the surface is given by

\[ \Pi = \frac{S_w \times S_v}{\| \Pi \|} \]  

(20)

for each \((w, v)\) point, and the second fundamental form is defined as the quadratic form

\[ \Pi = Lw^2 + 2Mwv + Nv^2 \]  

(21)

Where the coefficients \( L, M \) and \( N \) are defined as follows:

\[ L = S_{ww} \cdot \Pi; \quad M = S_{wv} \cdot \Pi; \quad N = S_{vv} \cdot \Pi \]  

(22)

\( \Pi \) approximates the perpendicular distance from the tangent plane to the point of surface fixed by \( S(w, v) \) for small values of \( w \) and \( v \). \( \Pi \) measures in the neighborhood of a point of tangency, the deviation of the surface from the tangent plane.

In order to find a more precise information, based on the fundamental forms and its coefficients, curvature measures have been proposed. The normal curvature can be thought as the rate of change of the direction of each curve over the surface; therefore, it is the quotient between the first two fundamental forms:

\[ k_n = \frac{\Pi}{I} \]

There is a pair of orthogonal directions for which \( k_n \) reach a maximum and minimum values, \( k_1 \) and \( k_2 \). They are called the principal curvature in a point \( p \).
The product between them is called the gaussian curvature \( K \), and its mean is called the mean curvature \( H \),

\[ K = k_1 k_2, \quad H = \frac{1}{2} (k_1 + k_2) \tag{23} \]

These are related with the first two fundamental forms through the next equivalences:

\[ K = \frac{LN - M^2}{EG - F^2}, \quad H = \frac{EN + LG - 2MF}{2(EG - F^2)} \tag{24} \]

### 4 Smoothness measures for surfaces

[10] proposed two smoothness measures, based on the curvatures and fundamental forms, for assessment of the quality of surface construction in computer graphics. Here, we use those measures in order to evaluate the smoothness of the surface generated by the covariance function, mainly near the origin and with this result, determine the characteristics of the associated random field.

The second-order smoothness is defined as

\[
\lambda(\|\mathbf{h}\|, u) = \left( \frac{1}{\pi} \int_0^{\pi} k_n^2(\alpha) d\alpha \right)^{1/2}
\]  

which integrates the square of the normal curvature for all directions on the tangent plane; therefore, it measures the trend of the function to bend itself. So, lower values appear when the function is smoother. The angle \( \alpha \) is measured from the first principal direction; \( k_n \) is a function of \( \alpha \) according to Euler’s formula:

\[ k_n(\alpha) = k_1 \cos^2 \alpha + k_2 \sin^2 \alpha. \]

There is a simpler way to calculate (25) in terms of the principal directions. Replacing Euler’s formula and by using (23), we have

\[
\lambda^2(\|\mathbf{h}\|, u) = \frac{3}{2} H^2 - \frac{1}{2} K \tag{26}
\]

and due to the equivalence , the second-order smoothness can be given in terms of its coefficients of fundamental forms,

\[
\lambda^2 = \frac{3G^2L^2 + (4M^2 + 2LN)(EG + 2F^2) + 3E^2N^2 - 12FM(EN + GL)}{8\sigma^4} \tag{27}
\]

which is an expression easier to compute.

Another option is the third-order smoothness [10], which corresponds to the total variation of the normal curvature at each point, in all directions of the tangent plane. This measure is defined as
\[ \Lambda(||h||, u) = \left( \frac{1}{\pi} \int_{0}^{\pi} (k'_u(\alpha))^2 \, d\alpha \right)^{1/2} \]  

which integrates the square of the variation over all possible directions. \( \Lambda(||h||, u) \) can be given in terms of the first fundamental form \( E, F, G \) and the coefficients \( P, Q, S, T \) which express the variation of the normal curvature in terms of the arc length:

\[
\begin{align*}
P &= \mathcal{S}_{ww} \cdot \mathbf{n} + 3 \mathcal{S}_{ww} \cdot \mathbf{n}_w \\
Q &= \mathcal{S}_{ww} \cdot \mathbf{n} + 3 \mathcal{S}_{ww} \cdot \mathbf{n}_w + \mathcal{S}_{ww} \cdot \mathbf{n}_w \\
S &= \mathcal{S}_{vv} \cdot \mathbf{n} + 2 \mathcal{S}_{vv} \cdot \mathbf{n}_v + \mathcal{S}_{vv} \cdot \mathbf{n}_v \\
T &= \mathcal{S}_{vv} \cdot \mathbf{n} + 3 \mathcal{S}_{vv} \cdot \mathbf{n}_v 
\end{align*}
\]

The easier way to calculate the third order smoothness, is replacing all coefficients to obtain:

\[
\Lambda^2 = \frac{1}{16\sigma^6} \left[ 5G^3P^2 + 5E^3T^2 + 9G(EG + 4F^2)Q^2 + 9E(EG + 4F^2)S^2 + 6(EG + 4F^2)(GPS + EQT) - 2F(3EG + 2F^2)(PT + 9QS) - 30F(G^2PQ + E^2ST) \right]
\]

This measure \( \Lambda \) shows the velocity of change of smoothness.

### 5 Results

The surface generated by the smoothness measures allows to determine the different levels of smoothness corresponding to each space-time lag and to detect the possible existence of ridges. The smoothness measure functions take its maximum values at the values of \( h \) and \( u \) for which the smoothness of the covariance function is lower, whereas they take the minimum values at the lags for which the covariance function is smoother. When these are ridges, we find a constant behavior.

#### 5.1 Spatial covariance functions

To illustrate the smoothness measures (25), it is initially applied to some cases in \( \mathbb{R}^2 \), see Figure 1.
• Covariance model of Matern. \( v > 0, \theta = (\sigma^2, a, v), a > 0 \)

\[
C(h) = \frac{\sigma^2}{2^{v-1} \Gamma(v)} (\|h\|/a)^v K_v(\|h\|/a)
\]

respectively, where \( K_v(\cdot) \) is the modified bessel function of order \( v \). This model is valid given that \( v > 0 \). The parameter \( v \) is a shape parameter which determines the analytic smoothness of the underlying process, [11].

• If \( v = \frac{1}{2} \) the Matern model agrees with the **Exponential model**

\[
C(h) = \sigma^2 \exp\{-\|h\|/a\}
\]

• When \( v \to \infty \) the limit case of Matern model is called the **Gaussian model**

\[
C(h) = \sigma^2 \exp\{- (\|h\|/a)^2\}
\]

Fig. 1 Second order smoothness for spatial Exponential and Gaussian covariance models.
The $\lambda$ function of an exponential model, shows lack of smoothness near the origin and higher smoothness as $\|h\|$ increases. That is, the exponential covariance model is not smooth at the beginning and reaches its maximum smoothness gradually. This is the ideal behavior of smoothness for a covariance model according to [3]. The maximum value and the $\|h\|$-value corresponding depend on $a$ and $\sigma$. For the other hand, the spatial Gaussian covariance model reaches its minimum smoothness at the origin, when its lambda function takes the maximum. The lambda function for this model, has a zero when $h = \pm \frac{a}{\sqrt{2}}$, that is, at this point there is a maximum smoothness, and then starts to grow up, reaching a local maximum before reaching again highest smoothness. So, the Gaussian covariance is not smoother away from the origin than near the origin. These behaviors are generalized in the Matern function, see Figure 2 until $\nu = 0.5$, the behavior is the same like the exponential, and for $\nu > 0.5$ the behavior is like the Gaussian. Then, for $\nu > 0.5$ the underlying processes have to be measured continuously, which in general, cannot be done in the practice, and the observations which strongly affect the prediction, are inside a too small neighborhood from the origin. Besides, the observations with a lag around the local maximum have more importance than others, which are nearest to the origin. Those are the processes that [3] considers unrealistic from a physical point of view.

5.2 Space-time covariance functions

For space-time covariance functions, $\mathcal{S}$ corresponds to the surface associated with

$$C(\|h\|, \tau) : \mathbb{R}^2 \rightarrow \mathbb{R}$$

and the parametrization used is

$$\left(\|h\|, \tau, C(\|h\|, \tau)\right)$$ (32)

The interest is to determine if the covariance function near to the origin is as smooth as away from the origin, or if the function has ridges. The space-time
Exponential and Gaussian models, have the same properties than their marginal functions in each of the axes. See Figure 3. These models are given by

\[
C(\|h\|, u) = \sigma^2 \exp \left\{ -\frac{\|h\|}{a} - \frac{u}{b} \right\} \quad \text{and} \quad C(\|h\|, u) = \sigma^2 \exp \left\{ -\left( \frac{\|h\|}{a} \right)^2 - \left( \frac{u}{b} \right)^2 \right\}
\]

where \(\sigma^2 > 0\) is the variance of space-time process; \(a > 0\) and \(b > 0\) are the parameters of space and time, respectively.

\[
\text{Exp}(\sigma = a = b = 1) \quad \text{Exp}(\sigma = 1, a = 0.1, b = 1) \quad \text{Gauss}(\sigma = 4, a = 1, b = 1) \quad \text{Gauss}(\sigma = 4, a = 1, b = 2)
\]

Fig. 3 Second order smoothness for space-time Exponential and Gaussian covariance models.

The behavior of the covariance families in [1], examples 1, 2 and 3, have ridges for some combinations of parameters, in a similar way than the Gaussian covariance. However, the smoothness of example 4 in [1], is like the exponential model. The Gneiting covariance models, [2], have basically two kinds of behaviors as we can observe in Figure 4. This is the second order smoothness for the Gneiting model obtained when the functions in 34 are \(\varphi\) and \(\phi\) in Theorem 2,

\[
\varphi(r) = e^{(-cr)} \quad \text{and} \quad \phi(r) = (1 + ar^\alpha)^\beta
\]

with \(c > 0\), \(a > 0\), \(0 < \gamma \leq 1\), \(0 < \alpha \leq 1\) and \(0 \leq \beta \leq 1\). The resulting covariance parametric family is

\[
C(h, u) = \frac{\sigma^2}{(1 + au^\alpha)^\beta \gamma} e^{\frac{-c\|h\|^\gamma}{(1 + au^\alpha)^\beta}}
\]

where \(a \gamma c\) (nonnegatives) are scaling parameters of time and space, respectively. The \(\alpha\) and \(\gamma\) parameters control the smoothness of function and the parameter \(\beta\) corresponds to the space-time interaction; \(\sigma^2\) is the variance of space-time process.

The function is smoother at the origin than away the origin 4a., or the second behavior is observed in 4b. and 4c. where although the smoothness is increasing from the origin, only has variation in an infinitesimal neighborhood of the origin, and then is constant. Notice that the plot in 4c. is made for a very small lags.
Fig. 4 Second order smoothness for space-time Gneiting covariance models. \( \gamma \) is the interaction parameter

6 Conclusions

The smoothness functions \( \lambda \) allow to identify the maximum distance to which the observations have strong effect on the prediction. In addition, when the covariance function has ridges, observations away from the origin can have much influence on the prediction. Then, first of all, it is necessary to determine if the underlying process can have the continuity that the covariance model implies, and secondly evaluates the real possibility to observe that process. In other cases, the weights in the prediction only correspond to lags with negligible effect on the prediction. We include here the most known covariance functions and it was enough to illustrate the different kinds of behavior. However, the only requirements to use the smoothness measures is the existence of the second derivate of covariance functions. The calculations and graphs were made with the software R and Mathematica 8.0.

References