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ORIGINAL PAPER

Revised and wider classes of isotropic space-time covariance functions

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Abstract

Several classes of space-time correlation models have been proposed by various authors in the last years. However, most of these families utilize non negative covariance functions to be adapted to different case studies: indeed, the traditional classes of covariances, such as the Whittle–Matern class and the several families constructed by applying the classical properties are not so flexible to describe covariance functions characterized by negative values. A recent analysis, regarding the difference between two isotropic covariance functions, has underlined that these new families of models are more flexible than the traditional ones because the same models are able to select covariance functions which are always positive in their domain, as well as covariance functions which could be negative in a subset of their field of definition. Moreover, within the same class of models, it is possible to select covariance models which present different behaviours in proximity of the origin. In this paper several families of isotropic space-time covariance functions, among the ones proposed in the literature, have been reviewed in order to enrich the same families including models characterized by negative values in a subset of their domain. Furthermore, the definition of separability has been revised in order to enlarge the classical definition. Apart from the theoretical importance related to the new aspects, these new classes of covariance models are characterized by an extremely simple formalism and can be easily adapted to several case studies.

Keywords Separable covariance functions · Non separable covariance functions · Negative correlation

1 Introduction

In the last 30 years a wide list of families of space-time covariance functions have been proposed by various authors: a detailed and comprehensive review has been provided in Porcu et al. (2021). However, selecting an appropriate class of models for a variable under study is still difficult and it represents a priority problem with respect to the choice of a particular model of a specified class. Several important characteristics have to be considered in order to select an appropriate class of space-time covariances, such as variability in space and in time, behavior at the origin, non separability, effect of interaction parameters, asymptotic behavior and anisotropy aspects. However, most of the families of space-time covariance functions proposed in the literature are positive: this important aspect can also be explicitely detected in all the examples proposed in many branches of applied sciences, such as in Atmospheric Sciences (Brown et al. 2001), in Environmental Sciences (De Cesare et al. 2001b), in Meteorology (Bourotte et al. 2016; Cressie and Huang 1999; Gneiting 2002), in Machine learning (Garg et al. 2018), in Forestry (Jost et al. 2005), in Demography (De Iaco et al. 2015) and in Finance (Porcu et al. 2012). This same feature characterizes the Whittle–Matern class (Matérn 1980; Hristopulos 2020): as a consequence a negative correlation cannot be modelled from the above set of covariances. Indeed, many applications concerning phenomena related to turbolence in space-time, biology and hydrology, require covariance functions with negative values, as described by some authors (Levinson et al. 1984; Yakhot et al. 1989; Shkarofsky 1968; Pomeroy et al. 2003; Xu et al. 2003a, b).

For what concerns correlation models characterized by negative values, a special family of infinitely differentiable Bessel–Lommel covariance functions that always exhibit a negative hole effect and are valid in $\mathbb{R}^n$, where $n > 2$, was

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derived by Hristopulos (2015), although the exact functional form of these covariance functions is not exactly the same for different dimensions. Moreover, a special class of covariance functions (the generalized sum of product models), characterized by negative weights, has been analyzed by Gregori et al. (2008).

An interesting contribution concerning a new technique to construct positive definite functions from multiply monotone functions is given in Buhmann and Jager (2020). Moreover, the positive definiteness of the Zastavnyi operator for the Matern, Generalized Cauchy and Wendland families, acting on rescaled weighted difference between two positive definite radial functions, has been analyzed by Faouzi et al. (2020).

The permissibility for the linear combinations of two real spatial or spatio-temporal covariance functions (or variograms) isotropic in space, in all dimensions, has been investigated by Ma (2005). It was found out that the resultant covariance may be just available in certain finite dimensions if one of the coefficients of the linear combinations is negative.

The results given by Ma (2005) and Faouzi et al. (2020) are only valid for real covariance functions; however, a covariance is a complex valued function. The general problem concerning the difference of two covariance functions in the complex domain has been analyzed in Posa (2021). In the special case of real isotropic covariance functions, the results given in Ma (2005), concerning the linear combination of two spatial or spatio-temporal covariance functions, are valid in any dimensional space; some of the results for real covariance functions, given in Posa (2021), are special cases of Ma's results. However, details concerning the practical aspects and the behaviour of the difference between two covariance functions in $\mathbb{R}, \mathbb{R}^2$ and $\mathbb{R}^3$ have been discussed in Posa (2021, 2023).

Starting from the above theoretical results, some traditional families of space-time covariance functions have been reviewed, hence these new classes enrich the traditional models which are very often characterized just by positive values of the correlation function. In particular, wider classes of separable and non separable space-time covariance functions will be constructed, able to be adapted to several case studies, in order to include models characterized by negative values in a subset of their domain. In particular, negative correlation structures are important for problems of biological, medical and physical nature; empirical examples of negative spatial autocorrelation can be found in Griffith (2019) and Hu et al. (2018). It is important to point out that some special covariance families, proposed in the literature, cannot ever assume, by construction, negative values, such as the Gneiting class and Whittle–Matern class; moreover, it will be shown that even in the integrated product models the resulting space-time covariances could be always positive although the basic spatial and temporal models are negative in a subset of their domain.

Furthermore, the definition of separability/non-separability has been revised in order to enlarge the traditional definition (Rodrigues and Diggle 2010; De Iaco and Posa 2013).

This paper is organized as follows: in Sect. 2, an overview concerning traditional classes of space-time covariance functions is provided, together with the classical definition of separability which is valid only for positive covariance functions. Some well known models, often utilized in the applications, have been considered. Indeed, the whole family of positive covariance functions can be splitted in two disjoint sets: separable and non separable models; the most relevant properties and drawbacks of these classes have been underlined. In Sect. 3 some traditional classes of space-time covariance functions have been reviewed, in order to enrich the same families with models characterized by negative values in a subset of their domain; a peculiar parametric analysis on these families has been given. In Sect. 4 a graphical representation of the most significant results, which can be utilized in a flexible and easy way by many practitioners, has been provided. At last, as far as we know, classes of covariance functions, able to describe various and different scenarios as the ones presented in this paper, seem not to exist.

2 Overview of space-time covariance functions

In literature, different space-time covariance models are available and they are usually classified in two main categories: *separable* and *non-separable* space-time covariance models.

Measures of separability/non separability have been firstly introduced by Rodrigues and Diggle (2010) and then extended by De Iaco and Posa (2013); however, all these measures are valid only for positive covariance functions. A general definition of separability/non separability will be successively provided in Sect. 3 and valid for any covariance function.

2.1 Definition of separability/non separability

As already pointed out, in the literature measures of separability/non separability have tacitly been given for positive covariance functions; these measures are recalled hereafter.

Definition 1 Let $C(\mathbf{x}, t, \mathbf{\Theta}) > 0, \forall (\mathbf{x}, t) \in S \times T \subseteq \mathbb{R}^n \times \mathbb{R}$, be a covariance function of a second order stationary space-time random field, where $\mathbf{\Theta}$ is a vector of parameters; let

$$\rho(\mathbf{x}, t; \mathbf{\Theta}) = \frac{C(\mathbf{x}, t; \mathbf{\Theta})}{C(\mathbf{0}, 0; \mathbf{\Theta})}$$

be the corresponding space-time correlation function, where $C(\mathbf{0}, 0; \mathbf{\Theta}) > 0$ and define the following ratio:

$$\begin{aligned} r(\mathbf{x}, t; \mathbf{\Theta}) &= \frac{\rho(\mathbf{x}, t; \mathbf{\Theta})}{\rho(\mathbf{x}, 0; \mathbf{\Theta})\rho(\mathbf{0}, t; \mathbf{\Theta})} \\ &= \frac{C(\mathbf{x}, t; \mathbf{\Theta})}{C(\mathbf{x}, 0; \mathbf{\Theta})} \cdot \frac{C(\mathbf{0}, 0; \mathbf{\Theta})}{C(\mathbf{0}, t; \mathbf{\Theta})}; \end{aligned} \tag{1}$$

analogously, the following difference $d(\mathbf{x}, t; \mathbf{\Theta})$ between $\rho(\mathbf{x}, t; \mathbf{\Theta})$ and $\rho(\mathbf{x}, 0; \mathbf{\Theta})\rho(\mathbf{0}, t; \mathbf{\Theta})$, can be defined, that is:

$$d(\mathbf{x}, t; \mathbf{\Theta}) = \rho(\mathbf{x}, t; \mathbf{\Theta}) - \rho(\mathbf{x}, 0; \mathbf{\Theta})\rho(\mathbf{0}, t; \mathbf{\Theta}), \tag{2}$$

or equivalently

$$d'(\mathbf{x}, t; \mathbf{\Theta}) = C(\mathbf{x}, t; \mathbf{\Theta})C(\mathbf{0}, 0; \mathbf{\Theta}) - C(\mathbf{x}, 0; \mathbf{\Theta})C(\mathbf{0}, t; \mathbf{\Theta}). \tag{3}$$

Then, the covariance C is *separable*, if:

$$\begin{aligned} &r(\mathbf{x}, t; \mathbf{\Theta}) = 1, \quad or \quad d(\mathbf{x}, t; \mathbf{\Theta}) = 0 \\ &\quad \forall (\mathbf{x}, t) \in S \times T, \forall \mathbf{\Theta}; \end{aligned} \tag{4}$$

moreover, the covariance C is *uniformly positive non separable*, if:

$$\begin{aligned} &r(\mathbf{x}, t; \mathbf{\Theta}) > 1, \quad or \quad d(\mathbf{x}, t; \mathbf{\Theta}) > 0 \\ &\quad \forall (\mathbf{x}, t) \in S \times T, (\mathbf{x}, t) \neq (\mathbf{0}, 0), \quad \forall \mathbf{\Theta}, \end{aligned} \tag{5}$$

or alternatively it is *uniformly negative non separable*, if:

$$\begin{aligned} &r(\mathbf{x}, t; \mathbf{\Theta}) < 1, \quad or \quad d(\mathbf{x}, t; \mathbf{\Theta}) < 0 \\ &\quad \forall (\mathbf{x}, t) \in S \times T, (\mathbf{x}, t) \neq (\mathbf{0}, 0), \quad \forall \mathbf{\Theta}. \end{aligned} \tag{6}$$

On the other hand, if $r(\mathbf{x}, t; \mathbf{\Theta}) > 1$ or $d(\mathbf{x}, t; \mathbf{\Theta}) > 0$ for some $(\mathbf{x}, t; \mathbf{\Theta})$, then the covariance function is pointwise positive non separable at $(\mathbf{x}, t; \mathbf{\Theta})$; alternatively, it is pointwise negative non separable at $(\mathbf{x}, t; \mathbf{\Theta})$, if $r(\mathbf{x}, t; \mathbf{\Theta}) < 1$ or $d(\mathbf{x}, t; \mathbf{\Theta}) < 0$ for some $(\mathbf{x}, t; \mathbf{\Theta})$. Hence, depending on the values of the parameter vector $\mathbf{\Theta}$ or the lag vector $(\mathbf{x}, t)$, the type of non separability for a given class of covariance functions might change.

Alternatively, the covariance function is *separable* if there exist spatial and temporal covariance functions C_S and C_T, respectively, such that

$C(\mathbf{x}, t; \mathbf{\Theta}) = C_S(\mathbf{x}; \mathbf{\Theta})C_T(t; \mathbf{\Theta})$, or equivalently

$$C(\mathbf{x}, t; \mathbf{\Theta}) = \frac{C(\mathbf{x}, 0; \mathbf{\Theta})C(\mathbf{0}, t; \mathbf{\Theta})}{C(\mathbf{0}, 0; \mathbf{\Theta})}. \tag{7}$$

hence by setting $r(\mathbf{x}, t; \mathbf{\Theta}) = 1$ in Eq. (1), if the covariance function is separable, then the correlation function is the product of the spatial and temporal marginals $\rho(\mathbf{x}, 0; \mathbf{\Theta})$ and $\rho(\mathbf{0}, t; \mathbf{\Theta})$. Equivalently, the sign of (2) and (3) will give information about the kind of non-separability: in particular, if a covariance function is separable, then $d(\mathbf{x}, t; \mathbf{\Theta}) = d'(\mathbf{x}, t; \mathbf{\Theta}) = 0$. Considering the above definitions, interesting results have been given in De Iaco and Posa (2013).

In the literature, separability can be checked through several statistical tests (Cappello et al. 2018; Gneiting et al. 2007; Li et al. 2007; Scaccia and Martin 2005; Mitchell et al. 2005). If the hypothesis of separability is rejected, then a non separable covariance model is required.

Remarks

- Note that expression (1) is equivalent to expressions (2) and (3) if and only if the covariance function $C(\mathbf{x}, t, \mathbf{\Theta}) > 0, \forall (\mathbf{x}, t) \in S \times T$; indeed, expression (1) is not defined if the marginals $C(\mathbf{x}, 0; \mathbf{\Theta})$ and $C(\mathbf{0}, t; \mathbf{\Theta})$ are continuous covariance functions which are negative in a subset of their domain: infact, in this case, there always exists at least one point in which these marginals are zero.
- Although the above definition of separability is particularly relevant for positive space-time covariance functions, it can be easily extended to any positive covariance function; in particular, a positive covariance function $C(\mathbf{s})$, defined in $\mathbb{R}^n$, is separable if there exist $n_1 \in \mathbb{N}$ and $n_2 \in \mathbb{N}$, with $n_1 + n_2 = n$ such that:

  $$C(\mathbf{s}) = C_1(\mathbf{s}_1)C_2(\mathbf{s}_2), \quad \mathbf{s} = (\mathbf{s}_1, \mathbf{s}_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2},$$

  where C_1 is a covariance function defined in $\mathbb{R}^{n_1}$ and C_2 is a covariance function defined in $\mathbb{R}^{n_2}$, with $\mathbb{R}^n = \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$. In what follows, the dependence on the vector of parameters $\mathbf{\Theta}$ will be omitted if not explicitely required.

2.2 Separable space-time covariance functions

As previously described, a space-time covariance function is *separable* if the non separability ratio $r(\mathbf{x}, t) = 1$ or equivalently the non separability index $d(\mathbf{x}, t; \mathbf{\Theta}) = d'(\mathbf{x}, t) = 0$.

The *product model* is the only model which belongs to this category; it is known in two versions: the one obtained by the product of purely spatial and purely temporal covariances (Rouhani and Myers 1990; Posa 1993), i.e.,

$$C(\mathbf{x}, t) = C_S(\mathbf{x})C_T(t),$$

and the other one where the global variance is multiplied by a purely spatial correlation function and a purely temporal correlation function (Haas 1995), i.e.,

$$C(\mathbf{x}, t) = \sigma^2 \rho_S(\mathbf{x}) \rho_T(t), \tag{8}$$

where $\sigma^2 = C(\mathbf{0}, 0)$ is the variance, ρ_S is the spatial correlation function and ρ_T is the temporal correlation function.

It is well known that the separable space-time covariance model has been one of the first attempts to describe spatio-temporal phenomena, because of its simple expression, however models of this type do not allow for space-time interaction.

The separable model (8) is just suitable to model the correlation of spatio-temporal random fields characterized by the same spatial and temporal variance. Hence, if the purely spatial and purely temporal correlation models of (8) decay at infinity, then

$$\forall\, t, \lim_{\|\mathbf{x}\| \to \infty} C(\mathbf{x}, t) = 0; \qquad \forall\, \mathbf{x}, \lim_{|t| \to \infty} C(\mathbf{x}, t) = 0.$$

At last, the separable model is integrable in space-time if ρ_S and ρ_T are integrable functions.

2.3 Non separable space-time covariance functions

All covariance models, different from the separable product model, characterize this class. In Porcu et al. (2021) the class of non separable covariance functions has been classified according to the following scheme:

- scale mixtures, such as the quasi-arithmetic class (Porcu et al. 2009), the models proposed by Fonseca and Steel (2011), Apanasovich et al. (2012), Porcu et al. (2007), Cressie and Huang (1999), the integrated product and product-sum models (De Iaco et al. 2002);
- classes obtained by applying the properties of positive-definite functions seen as convex cone, such as the sum model (Rouhani and Hall 1989), the product-sum models (De Cesare et al. 2001a), Rodrigues and Diggle models (Rodrigues and Diggle 2010) and models generated by mixtures (Ma 2002, 2003);
- spectral density approaches, proposed by Stein (2005) and Posa (2021);
- lagrangian reference frame, whose covariance functions are no longer fully symmetric (Cox and Isham 1988; Gneiting et al. 2007);
- classes with special features (Christakos and Hristopoulos 1998; Kolovos et al. 2004; Brown et al. 2000).

Indeed, most of the previous families of covariance functions (Porcu et al. 2009; Cressie and Huang 1999; Ma 2002, 2003; Rouhani and Hall 1989; Rodrigues and Diggle 2010; De Cesare et al. 2001a; De Iaco et al. 2002) have been built utilizing the combined result of the Kronecker product between the spatial and the temporal marginals and the classical properties of covariance functions.

A brief overview concerning the most utilized space-time non separable covariance models, with their properties and shortcomings is presented hereafter, in order to provide an exhaustive overview and a comparative analysis. Please note that the same analysis can be drawn for some other classes of space-time covariance models which have not explicitely analyzed in this paper.

2.3.1 The sum model

The *sum model* (Rouhani and Hall 1989), also called zonal anisotropy model, is obtained by the sum of purely spatial and purely temporal covariances:

$$C(\mathbf{x}, t) = C_S(\mathbf{x}) + C_T(t), \tag{9}$$

C_S and C_T are, respectively, purely spatial and purely temporal covariance models.

The family of covariance functions defined in (9) has been wrongly included within the class of separable models (Cressie and Huang 1999). Indeed, according to definition (1) and (3), in the following it is shown that the sum model is characterized by negative non separability, as a consequence it cannot be considered *separable*.

Corollary 1 *The sum model, defined in Eq. (9), is non separable.*

Proof (See the Appendix). □

According to the previous result, the sum model is *uniformly negative non separable*, hence it cannot model correlation structures characterized by positive non separability; moreover, the same model is not strictly positive definite even if C_S and C_T are strictly positive definite correlation functions (De Iaco and Posa 2018). At last, the sum model is not integrable in space-time even if C_S and C_T are integrable functions, hence in the Bochner representation it cannot be expressed through a spectral density function.

2.3.2 The product-sum model

In the product-sum model (De Cesare et al. 2001a, b)

$$\begin{aligned} &C(\mathbf{x}, t) = k_1 C_S(\mathbf{x}) C_T(t) + k_2 C_S(\mathbf{x}) + k_3 C_T(t), \\ &\quad k_1 > 0, k_2 \geq 0, k_3 \geq 0, \end{aligned} \tag{10}$$

C_S and C_T are, respectively, purely spatial and purely temporal covariance models.

Concerning the asymptotic behavior of the product-sum covariance model, if the purely spatial and purely temporal covariances are such that:

$$\lim_{\|\mathbf{x}\|\to\infty} C_S(\mathbf{x}) = \lim_{|t|\to\infty} C_T(t) = 0,$$

then

$$\forall t, \lim_{\|\mathbf{x}\|\to\infty} C(\mathbf{x},t) = k_3 C_T(t); \quad \forall \mathbf{x}, \lim_{|t|\to\infty} C(\mathbf{x},t) = k_2 C_S(\mathbf{x}).$$

Of course, if the limits on space and time exist and converge to values which are generally different, the following limit $\lim_{\|(\mathbf{x},\mathbf{t})\|\to\infty} C(\mathbf{x},t)$ does not exist.

Note that the product-sum model does not decay at infinity along the spatial and temporal axes, then it enables to model different variabilities along space and time, as it can be seen by setting $t = 0$ in the first limit and $\mathbf{x} = \mathbf{0}$ in the second one. On the other hand, the class (10) cannot model space-time processes characterized by the same variability along space and time. Assuming that $C_S(\mathbf{x}) > 0 \quad \forall \mathbf{x}$ and $C_T(t) > 0 \quad \forall t$, the index d' defined in (3) can be easily computed:

$$d'(\mathbf{x},t) = k_2 k_3 \left[C_T(0) - C_T(t)\right]\left[C_S(\mathbf{x}) - C_S(\mathbf{0})\right] < 0; \tag{11}$$

hence the product-sum covariance models can just describe stationary space-time covariances that are uniformly negative non separable. Even in this case, the above index can be equivalently written as follows: $d'(\mathbf{x},t) = -k_2 k_3 \gamma_S(\mathbf{x})\gamma_T(t)$, where γ_S and $\gamma_T(t)$ are the spatial marginal and temporal marginal semivariogram, respectively. At last, the product-sum model is not integrable in space-time even if C_S and C_T are integrable functions, hence in the Bochner representation it cannot be expressed through a spectral density function.

2.3.3 The integrated product-sum model

The integrated product-sum model (De Iaco et al. 2002) in terms of the spatio-temporal correlation function:

$$\rho(\mathbf{x},t) = \int_V \Big[k_1 \rho_S(\mathbf{x};\alpha)\rho_T(t;\alpha) + k_2 \rho_S(\mathbf{x};\alpha) + k_3 \rho_T(t;\alpha)\Big] d\mu(\alpha), \tag{12}$$

where μ is a positive measure on $U \subseteq \mathbb{R}$, ρ_S and ρ_T are correlation functions defined on $D \subseteq \mathbb{R}^n$ and $T \subseteq \mathbb{R}$, respectively, for all $\alpha \in V \subseteq U$, $k_1 > 0$, $k_2 \geq 0$ and $k_3 \geq 0$, $k_1 + k_2 + k_3 = 1$ and $\int_V d\mu(\alpha) = 1$; let

$$a = \int_V [\rho_S(\mathbf{x};\alpha)\rho_T(t;\alpha)] d\mu(\alpha), \quad b = \int_V [\rho_S(\mathbf{x};\alpha)] d\mu(\alpha),$$
$$c = \int_V [\rho_T(t;\alpha)] d\mu(\alpha).$$

Then the difference (2) can be easily obtained:

$$d(\mathbf{x},t) = ak_1 + bk_2 + ck_3 - [(k_1 + k_2)b + k_3][(k_1 + k_3)c + k_2],$$

which can be further simplified as follows:

$$d(\mathbf{x},t) = (a - bc)k_1 - (1-b)(1-c)k_2 k_3. \tag{13}$$

The sign of d might be positive or negative depending on the coefficients k_1, k_2 and k_3 (with 2 degrees of freedom) and the factor $(a - bc)$, or equivalently the sign of d depends on the inequality existing between $(a - bc)/[(1-b)(1-c)]$ and $k_2 k_3 / k_1$. If the factor $(a - bc)$ is negative, the above difference is always negative, for any k_1, k_2 and k_3. Note that $(a - bc)$ corresponds to the difference between the integrated product model and the product of the integrals of the same correlation functions. If the factor $(a - bc)$ is positive, the above difference might be positive and negative, according to the coefficients k_1, k_2 and k_3. It is worth noting that if $\rho_S(\cdot;\alpha)$ and $\rho_T(\cdot;\alpha)$ are both non-decreasing functions (or all are non-increasing functions) with respect to α, the factor $(a - bc)$ is always positive.

According to the previous rsults, the class of integrated product-sum covariance models can handle any form of non separability: uniformly positive and negative non separability and non uniformly non separability. Given a correlation model as in (12), if the purely spatial and purely temporal correlations are such that:

$$\lim_{\|\mathbf{x}\|\to\infty} \rho_S(\mathbf{x};\alpha) = \lim_{|t|\to\infty} \rho_T(t;\alpha) = 0,$$

then for the class of models (12):

$$\forall\, t, \lim_{\|\mathbf{x}\|\to\infty} \rho(\mathbf{x},t) = \int_V [k_3 \rho_T(t;\alpha)] d\mu(\alpha);$$
$$\forall\, \mathbf{x}, \lim_{|t|\to\infty} \rho(\mathbf{x},t) = \int_V [k_2 \rho_S(\mathbf{x};\alpha)] d\mu(\alpha).$$

These last results are proved by using the previous results on the product-sum model and by recalling the dominated convergence theorem in order to exchange limit and integral.

Setting $t = 0$ in the first limit and $\mathbf{x} = \mathbf{0}$ in the second one, the following results for the marginal covariances can be obtained:

$$t = 0, \lim_{\|\mathbf{x}\| \to \infty} \rho(\mathbf{x}, 0) = \int_V [k_3 \rho_T(0)] d\mu(\alpha);$$
$$\mathbf{x} = \mathbf{0}, \lim_{|t| \to \infty} \rho(\mathbf{0}, t) = \int_V [k_2 \rho_S(\mathbf{0}; \alpha)] d\mu(\alpha).$$

According to the previous results, the integrated product-sum models present essentially the same asymptotic behavior of the product-sum model, then it enables to model different variabilities along space and time. However, the class (12) cannot model space-time processes characterized by the same variability along space and time.

2.3.4 The integrated product model

If $k_2 = k_3 = 0$ in (12), the integrated product model is obtained:

$$\rho(\mathbf{x}, t) = \int_V \rho_S(\mathbf{x}; \alpha) \rho_T(t; \alpha) d\mu(\alpha). \tag{14}$$

Although the product model is separable, the integrated product is non separable; several examples can be found in De Iaco et al. (2002).

Assuming that $\rho_S(\mathbf{x}) \geq 0 \quad \forall \mathbf{x}$ and $\rho_T(t) \geq 0 \quad \forall t$, the difference (2) can be easily obtained:

$$d(\mathbf{x}, t) = a - bc, \tag{15}$$

where the parameters a, b and c have been previously defined; as a consequence, the class of integrated product covariance models, as a special case of (12), can handle any form of non separability: uniformly positive and negative non separability and non uniformly non separability.

Given a correlation model as in (14), if the purely spatial and purely temporal correlations are such that: $\lim_{\|\mathbf{x}\| \to \infty} \rho_S(\mathbf{x}; \alpha) = \lim_{|t| \to \infty} \rho_T(t; \alpha) = 0$, there always exists an integrable function G, with respect to the measure μ, which dominates the class of functions $\rho_S(\mathbf{x}; a) \rho_T(t; \alpha)$, that is: $|\rho_S(\mathbf{x}; \alpha) \rho_T(t; \alpha)| \leq G(\alpha), \forall (\mathbf{x}, t)$, because any correlation function is bounded, then for the class of models (14):

$$\forall\, t, \lim_{\|\mathbf{x}\| \to \infty} \rho(\mathbf{x}, t) = 0; \qquad \forall\, \mathbf{x}, \lim_{|t| \to \infty} \rho(\mathbf{x}, t) = 0.$$

Similarly to the product model, the integrated product model decays at infinity along the spatial and temporal axes, hence this class of models cannot handle space-time processes which present different variability along space and time.

2.3.5 Cressie–Huang class of models

In the Cressie–Huang class of models (Cressie and Huang 1999)

$$C(\mathbf{x}, t) = \int_{\mathbb{R}^n} e^{i\mathbf{x}^{\mathrm{T}}\boldsymbol{\omega}} \rho(t; \boldsymbol{\omega}) k(\boldsymbol{\omega}) d\boldsymbol{\omega}, \tag{16}$$

$\rho(\cdot; \boldsymbol{\omega})$ is a continuous integrable correlation function for all $\omega \in \mathbb{R}^n$, and $k(\cdot)$ is a positive function, which is integrable on $\mathbb{R}^n$. Although this class of models allows for space-time interaction, the same class is restricted to a small family of functions for which a closed form solution to the Fourier integral is known. Since the complex exponential can be written as: $e^{i\mathbf{x}^{\mathrm{T}}\omega} = cos(\mathbf{x}^T \boldsymbol{\omega}) + isin(\mathbf{x}^T \boldsymbol{\omega})$, if $\rho(\boldsymbol{\omega}; t) k(\boldsymbol{\omega})$ is symmetric about the origin in $\mathbb{R}^n$, then Cressie–Huang representation can be viewed as a special case of (14). Hence,

$$C(\mathbf{x}, t) = \int_{\mathbb{R}^n} e^{i\mathbf{x}^{\mathrm{T}}\boldsymbol{\omega}} \rho(\boldsymbol{\omega}; t) k(\boldsymbol{\omega}) d\boldsymbol{\omega}$$
$$= \int_{\mathbb{R}^n_+} C_S(\mathbf{x}; \boldsymbol{\omega}) C_T(t; \boldsymbol{\omega}) k(\boldsymbol{\omega}) d\boldsymbol{\omega},$$

where k is defined, positive and integrable over $\mathbb{R}_+$, $C_S(\mathbf{x}; \boldsymbol{\omega})$ is only positive semi-definite spatial covariance function for each $\boldsymbol{\omega} \in \mathbb{R}^n_+$ and C_T is a temporal covariance.

Recalling the existence of the spectral density of C, the Cressie–Huang class of models (16) is characterized by the following asymptotic behavior

$$\lim_{\|(\mathbf{x}, \mathbf{t})\| \to \infty} C(\mathbf{x}, t) = 0; \qquad \forall\, t, \lim_{\|\mathbf{x}\| \to \infty} C(\mathbf{x}, t) = 0;$$
$$\forall\, \mathbf{x}, \lim_{|t| \to \infty} C(\mathbf{x}, t) = 0.$$

From these results, it follows that this class of models is not suitable to describe phenomena characterized by a different variability in space and time.

Assuming that $C_S(\mathbf{x}) > 0 \quad \forall \mathbf{x}$ and $C_T(t) > 0 \quad \forall t$ and recalling that (16) can be viewed as a special case of (14), Cressie–Huang class is flexible enough to handle either uniformly positive and negative non separability.

2.3.6 Gneiting class of models

In the Gneiting class of models (Gneiting 2002)

$$C(\mathbf{x}, t) = \frac{\sigma^2}{[\psi(t^2)]^{n/2}} \phi\left(\frac{\|\mathbf{x}\|^2}{\psi(t^2)}\right), \tag{17}$$

$\mathbf{x} \in \mathbb{R}^n$, $\phi(t), t \geq 0$, is a completely monotone function and $\psi(t), t \geq 0$, is a positive function with completely monotone derivative; hence, the above class of models is always positive, as a consequence it cannot model space-time correlation structures characterized by negative values. Concerning the asymptotic behavior of the Gneiting class of models (17), two different cases can be mentioned, depending on the hypothesis on ψ.

Firstly, if $\lim_{t \to \infty} \psi(t) = \infty$, then:

1. $\forall\, t, \quad \lim_{\|\mathbf{x}\|\to\infty} C(\mathbf{x}, t) = 0$ (since ϕ vanishes at infinity by definition);
2. $\forall\, \mathbf{x}, \quad \lim_{|t|\to\infty} C(\mathbf{x}, t) = 0$ (from the hypothesis on ψ).

In this case, the class (17) cannot describe space-time processes which present different variability along space and time.

Secondly, given a covariance as in (17), if $\lim_{t\to\infty} \psi(t) = k$, then:

1. $\forall\, t, \quad \lim_{\|\mathbf{x}\|\to\infty} C(\mathbf{x}, t) = 0$ (since ϕ vanishes at infinity by definition);
2. $\forall\, \mathbf{x}, \quad \lim_{|t|\to\infty} C(\mathbf{x}, t) = \frac{\sigma^2}{k^{n/2}} \phi\left(\frac{\|\mathbf{x}\|^2}{k}\right)$ (from the hypothesis on ψ).

In this case the class (17) is not integrable in space-time and can describe space-time processes which present different variability along space and time. Note that for the marginal covariances, analogous results can be obtained from 1. and 2. by setting $t = 0$ in the first limit and $\mathbf{x} = \mathbf{0}$ in the second one. Hence, nothing can be said, in general, on the existence of the following limit $\lim_{\|(\mathbf{x},\mathbf{t})\|\to\infty} C(\mathbf{x}, t)$. For what concerns the type of non separability, the index d defined in (2), can be easily computed:

$$d(\mathbf{x}, t) = \frac{\sigma^2}{[\psi(t^2)]^{n/2}} \left[\phi\left(\frac{\|\mathbf{x}\|^2}{\psi(t^2)}\right) - \phi\left(\|\mathbf{x}\|^2\right)\right]; \tag{18}$$

since the function ϕ is decreasing and ψ is an increasing function with $\psi(0) = 1$, as a consequence $d(\mathbf{x}, t) > 0, \quad \forall\, \mathbf{x}, \forall\, t$.

According to the previous result, Gneiting class of covariance models is always characterized by uniform positive non separability, hence this class cannot model space-time processes characterized by negative non separability.

2.3.7 Rodrigues and Diggle class of models

Rodrigues and Diggle (2010) proposed the following space-time correlation model:

$$\rho(\mathbf{x}, t) = \frac{1}{2}\left(\rho_{S,1}(\mathbf{x})\rho_{T,1}(t) + \rho_{S,2}(\mathbf{x})\rho_{T,2}(t)\right), \tag{19}$$

where $\rho_{S,1}(\mathbf{x}), \rho_{S,2}(\mathbf{x}), \rho_{T,1}(t), \rho_{T,2}(t)$ are, respectively, two non negative and integrable spatial and two non negative and integrable temporal correlation functions. The integrability of the spatial and temporal correlation functions for the class (19) implies that:

$$\lim_{\|\mathbf{x}\|\to\infty} \rho_{S,i}(\mathbf{x}) = 0; \qquad \lim_{|t|\to\infty} \rho_{T,i}(t) = 0, \quad i = 1, 2,$$

as a consequence:

$$\forall\, t, \; \lim_{\|\mathbf{x}\|\to\infty} \rho(\mathbf{x}, t) = 0; \qquad \forall\, \mathbf{x}, \; \lim_{|t|\to\infty} \rho(\mathbf{x}, t) = 0.$$

From these results, it follows that the class of models (19) is not appropriate to describe phenomena characterized by a different variability in space and time.

Assuming that all the correlation models $\rho_{S,1}, \rho_{S,2}, \rho_{T,1}$ and $\rho_{T,2}$ be positive, the index d defined in (2) can be easily computed:

$$d(\mathbf{x}, t) = \frac{1}{4}\left(\rho_{S,1}(\mathbf{x}) - \rho_{S,2}(\mathbf{x})\right)\left(\rho_{T,1}(t) - \rho_{T,2}(t)\right), \tag{20}$$

hence Rodrigues and Diggle class of models is flexible enough to handle either uniformly positive and negative non separability suitably choosing the correlation models $\rho_{S,1}, \rho_{S,2}, \rho_{T,1}$ and $\rho_{T,2}$.

Remarks

- The non separability index d' is essentially the same for the sum and product-sum models, i.e. it is equal to minus the product of the spatial marginal and temporal marginal semivariograms. Indeed, the product-sum model can be considered a linear combination, with positive coefficients, of the sum model with a separable space-time correlation model, as a consequence, the non separability indexes are equivalent and they are always negative regardless of the spatial and temporal marginals correlation structures. Even for Gneiting family, the non separability index, which is always positive, does not depend on the correlation models utilized.
- On the other hand, the non separability index strongly depends on the spatial and temporal marginals for the integrated models, in particular for the Cressie–Huang class of models, and for the Rodrigues and Diggle family; for this last class of models, it is easy to check that the non separability index approaches to zero as the two spatial marginals (or the temporal marginals) become very close to each other.
- Cressie–Huang models, the product, the integrated product model and Rodrigues and Diggle models decay at infinity, namely, in terms of the corresponding variogram models, they reach the same sill value along space and time. Hence, these classes of covariances are not appropriate to model variables which do not present the same variability along space and time. On the other hand, the product-sum model, the integrated product-sum models and Gneiting models are able to model variables characterized by different variability along space and time.
- Cressie–Huang models, the integrated product, the integrated product sum models and Rodrigues and

Diggle models are flexible enough to handle either uniformly positive and negative non separability. On the other hand, the product sum models can only describe negative non separability, whereas Gneiting models are just characterized by positive non separability.

3 Wider classes of isotropic space-time covariance functions

The aim of the present Section is to revise some of the previous traditional classes of spatio-temporal covariance functions, which are isotropic in space, taking into account the main features, together with the drawbacks and limitations of the same classes. In particular, it can be underlined that:

- the Gneiting class of models, by construction, does not allow to model covariance functions characterized by negative values;
- all the examples proposed by the families of covariance functions of the previous Section in the various case studies, treat only positive covariance models; at this purpose, see for example, the applications proposed in Brown et al. (2001), De Cesare et al. (2001b), Bourotte et al. (2016), Cressie and Huang (1999), Gneiting (2002), Garg et al. (2018), Jost et al. (2005), De Iaco et al. (2015) and Porcu et al. (2012);
- for the family of models proposed by Rodrigues and Diggle (2010), all the correlation functions in (19) are assumed to be positive and integrable by the same authors;
- utilizing the well known properties and considering standard covariance models (see, for example, Whittle–Matern family, the rational and spherical models) it is not possible to generate covariances which can assume negative values;
- Yaglom (1987) presented oscillatory covariance functions utilizing some Bessel functions. Linear combinations of covariance functions with some negative coefficients can be found in Gregori et al. (2008);
- on the other hand, it is relevant to point out that it is possible to construct three-parameter isotropic covariance functions which take negative values for a specific range of values of one parameter (rigidity coefficient), as it has been shown for the so-called Spartan covariance functions (Hristopulos and Elogne 2007). In addition, the Spartan covariance functions for values of the rigidity parameter greater than 2 are expressed as the difference between two functions (Hristopulos 2015);
- in order to model covariance structures which present negative values or damped oscillations, covariance functions resulting from the product of standard positive models with a cosine function have been often utilized. However, this kind of covariance functions present some severe limitations and are not able to describe different structures modifying the values of their parameters.

The theoretical results given in Posa (2021) will be properly utilized hereafter to enrich the family of isotropic space-time covariance functions; according to these last results, in the present Section some interesting consequences outcoming from these special classes of covariance functions will be given: in particular, the resulting covariance models present some relevant and interesting properties which are often required in the applications, hence they can be easily utilized in several case studies. Indeed, the class of models proposed hereafter, according to the values of the parameters on which the same class depends, could be positive or negative in a subset of their domain; moreover, the models could portray different behaviours near the origin. Note that the concept of isotropy just refers to the spatial Euclidean space.

The following result allows to define a class of covariance functions which is particularly flexible to be utilized in several case studies.

Theorem 1 *The following class of parametric functions*:

$$\rho(t;k) = \frac{1-kt^2}{(t^2+1)^3}, \tag{21}$$

is a correlation function in $\mathbb{R}$ if and only if: $-\frac{1}{5} \le k \le 3$.

Proof (See the Appendix). □

In Fig. 1 it is shown the behaviour of model (21). As specified in Theorem 1, this class of covariances, according to the previous values of parameters, presents a parabolic behaviour in proximity of the origin, moreover, according to the values of the parameter k, it can be always positive if $-\frac{1}{5} \le k \le 0$, and can assume negative values in a subset of its domain if $0 < k \le 3$.

3.1 Wider classes of separable space-time covariance functions

In the applications separable space-time covariance models have been utilized by choosing spatial and temporal marginals only characterized by positive values. In the present Section, it will be shown how to construct separable space-time covariance models also characterized by negative values, in order to enrich the same class of separable models.

For the family of the separable space-time covariance models defined in expression (8), i.e.,

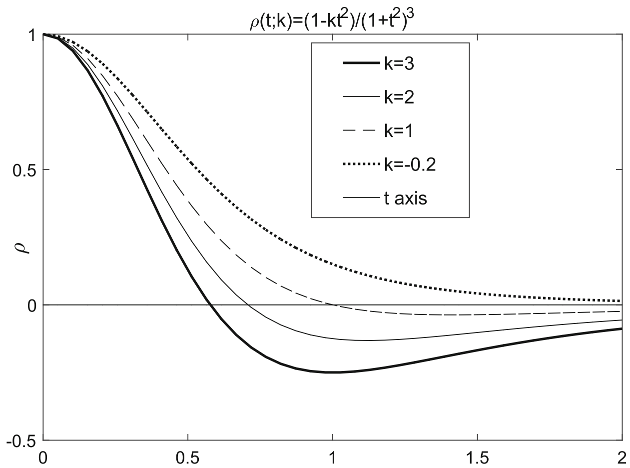

Fig. 1 Behaviour of model (21). It is always positive if $-\frac{1}{5} \le k \le 0$, and assumes negative values in a subset of its domain if $0 < k \le 3$

$$C(\mathbf{x}, t) = \sigma^2 \rho_S(\mathbf{x}) \rho_T(t),$$

the correlation functions ρ_S and ρ_T, can be chosen as follows (Posa 2021):

$$\rho_S(\mathbf{x}, A_1, A_2, \alpha_1, \beta_1) = A_1 \rho_1(\mathbf{x}, \alpha_1) - A_2 \rho_2(\mathbf{x}, \beta_1), \; A_1 - A_2 = 1, \tag{22}$$

$$\rho_T(t, B_1, B_2, \alpha_2, \beta_2) = B_1 \rho_3(t, \alpha_2) - B_2 \rho_4(t, \beta_2), \; B_1 - B_2 = 1, \tag{23}$$

or alternatively, according to Theorem 1:

$$\rho_T(t; \alpha) = \frac{1 - \alpha t^2}{(t^2 + 1)^3}, \quad -\frac{1}{5} \le \alpha \le 3,$$

hence the separable space-time covariance function C and the marginal correlations ρ_S and ρ_T can assume positive or negative values by properly choosing the parameters values. As already pointed out, an exhaustive parametric analysis on models (22) and (23) has been provided in Posa (2021). Note that all the results given in this last paper are valid for isotropic covariance functions. In particular, the spatial correlation functions ρ_1 and ρ_2 in (22) are supposed to be isotropic.

3.2 Wider classes of non separable space-time covariance functions

As previously outlined for separable models, in this Section some peculiar families of non separable covariance functions will be suitably enriched in order to obtain classes of space-time covariance functions characterized by negative values. In particular, for the various classes of non separable space-time covariance models described in Sect. 2, the only relevant models which allow for negative values regard the modified version of the class of the product-sum models and the revised class of Rodrigues and Diggle models, as specified hereafter.

3.2.1 Modified product-sum models

The product-sum model (10) introduced by De Cesare et al. 2001a, b, can be easily generalized as follows:

$$\begin{aligned} C(\mathbf{x}, t) =& k_1 C_{S,1}(\mathbf{x}) C_{T,1}(t) + k_2 C_{S,2}(\mathbf{x}) + k_3 C_{T,2}(t), \\ & k_1 > 0, k_2 \ge 0, k_3 \ge 0, \end{aligned} \tag{24}$$

$C_{S,i}$ and $C_{T,i}, i = 1, 2$ are, respectively, purely spatial and purely temporal covariance models. In the previous product-sum model (10) it is assumed that $C_{S,1} = C_{S,2} = C_S$ and $C_{T,1} = C_{T,2} = C_T$. Special cases of (24) are the following:

$$C(\mathbf{x}, t) = k_1 C_{S,1}(\mathbf{x}) C_{T,1}(t) + k_2 C_{S,2}(\mathbf{x}), \quad k_1 > 0, k_2 \ge 0, \tag{25}$$

and

$$C(\mathbf{x}, t) = k_1 C_{S,1}(\mathbf{x}) C_{T,1}(t) + k_2 C_{T,2}(t), \quad k_1 > 0, k_2 \ge 0. \tag{26}$$

In particular, in the previous classes (24), (25) and (26), the covariance functions $C_{S,\cdot}$ and $C_{T,\cdot}$, can be chosen as follows (Posa 2021):

$$\begin{aligned} &C_{S,\cdot}(\mathbf{x}, A_1, A_2, \alpha_1, \beta_1) = A_{1,\cdot} C_{1,\cdot}(\mathbf{x}, \alpha_1) - A_{2,\cdot} C_{2,\cdot}(\mathbf{x}, \beta_1), \\ &C_{T,\cdot}(t, B_1, B_2, \alpha_2, \beta_2) = B_{1,\cdot} C_{1,\cdot}(t, \alpha_2) - B_{2,\cdot} C_{2,\cdot}(t, \beta_2), \end{aligned}$$

or alternatively, according to Theorem 1:

$$C_{T,\cdot}(t; A, \alpha) = \frac{A - \alpha t^2}{(t^2 + 1)^3}, \quad -\frac{A}{5} \le \alpha \le 3A,$$

hence the non separable space-time covariance function C and the marginal covariances $C_{S,\cdot}$ and $C_{T,\cdot}$ can assume positive or negative values by properly choosing the parameters values.

The classes (25) and (26) can be equivalently written in terms of the spatial and temporal correlation functions, i.e.,

$$\begin{aligned} \rho(\mathbf{x}, t) =& A \rho_{S,1}(\mathbf{x}) \rho_{T,1}(t) + B \rho_{S,2}(\mathbf{x}), \\ & A > 0, B > 0, A + B = 1, \end{aligned} \tag{27}$$

$$\begin{aligned} \rho(\mathbf{x}, t) =& A \rho_{S,1}(\mathbf{x}) \rho_{T,1}(t) + B \rho_{T,2}(t), \\ & A > 0, B > 0, A + B = 1, \end{aligned} \tag{28}$$

and both models can assume negative values by choosing the correlation functions $\rho_{S,\cdot}$ and $\rho_{T,\cdot}$ as in (22) and in (23). The families (27) and (28) present interesting properties; if the spatial and temporal correlation functions are integrable, then for the class (27):

$$\forall\, t, \lim_{\|\mathbf{x}\|\to\infty} \rho(\mathbf{x},t) = 0; \qquad \forall\, \mathbf{x}, \lim_{|t|\to\infty} \rho(\mathbf{x},t) = B\rho_{S,2}(\mathbf{x}),$$

whereas for the class (28):

$$\forall\, t, \lim_{\|\mathbf{x}\|\to\infty} \rho(\mathbf{x},t) = B\rho_{T,2}(t); \qquad \forall\, \mathbf{x}, \lim_{|t|\to\infty} \rho(\mathbf{x},t) = 0.$$

In the peculiar case that the spatial and temporal correlation functions for the classes (27) and (28) are positive, the following results can be easily proved.

Corollary 2 *The non-separability index d for the class* (27) *is given by the following expression*:

$$d(\mathbf{x},t) = AB\left(1-\rho_{T,1}(t)\right)\left(\rho_{S,2}(\mathbf{x})-\rho_{S,1}(\mathbf{x})\right). \tag{29}$$

Proof The result can be easily obtained by applying definition (2). □

Corollary 3 *The non-separability index d for the class* (28) *is given by the following expression*:

$$d(\mathbf{x},t) = AB\left(1-\rho_{S,1}(\mathbf{x})\right)\left(\rho_{T,2}(t)-\rho_{T,1}(t)\right). \tag{30}$$

Proof The result can be easily obtained by applying definition (2). □

According to the previous Corollaries, the space-time correlation models (27) and (28) can handle both positive and negative non separability depending on the sign of $\left(\rho_{S,2}(\mathbf{x})-\rho_{S,1}(\mathbf{x})\right)$ and $\left(\rho_{T,2}(t)-\rho_{T,1}(t)\right)$, respectively.

3.2.2 A wider class of Rodrigues and Diggle models

In the class of models (19) proposed by Rodrigues and Diggle, the spatial and temporal correlation functions were assumed to be all positive. The same class of correlation models, defined by the authors, can be easily revised as follows:

$$\begin{aligned}\rho(\mathbf{x},t;\boldsymbol{\Theta}) =& A\rho_{S,1}(\mathbf{x};\theta_1)\rho_{T,1}(t;\phi_1)\\ &+B\rho_{S,2}(\mathbf{x};\theta_2)\rho_{T,2}(t;\phi_2), A>0, B>0, A+B=1,\end{aligned} \tag{31}$$

where $\rho_{S,1}(\mathbf{x};\theta_1), \rho_{S,2}(\mathbf{x};\theta_2), \rho_{T,1}(t;\phi_1), \rho_{T,2}(t;\phi_2)$ are, respectively, two valid and integrable spatial and two valid and integrable temporal correlation functions, not necessarily constrained to be positive, hence the non separable space-time correlation function ρ and the marginal correlations can assume positive or negative values by properly choosing the parameters values of the correlation functions $\rho_{S,\cdot}$ and $\rho_{T,\cdot}$ as in (22) and in (23) and the weights A and B.

Note that the modified product-sum models (27) and (28) cannot be considered special cases of model (31), because in this last class of models all the correlation functions involved are integrable, on the other hand the constant correlation functions $\rho_{T,2}(t)=1$ and $\rho_{S,2}(\mathbf{x})=1$ are not integrable. Moreover, with respect to the classical model given in (19), proposed by the authors in Rodrigues and Diggle (2010), in the class (31) the products $\rho_{S,i}\rho_{T,i}, i=1,2$ are suitably weighted through the parameters A and B.

3.3 Some notes on the integrated product models

As already pointed out, the families of space-time covariance models defined in (24), (25) and (26) can assume negative values by properly choosing the parameters values of the marginal spatial and temporal correlation structures on which they depend.

However, in the following Corollaries it will be shown that the family of the integrated product models, in which one of the marginals or both the marginals can assume negative values, the resulting space-time covariance is always positive in its domain. This result can also be applied to the Cressie–Huang class of models, because this last class can be viewed as a special case of the integrated product models, as already underlined.

Corollary 4 *Let*

$$C_S(x;a,A,B,\alpha,\beta) = Ae^{-a\alpha x} - Be^{-a\beta x}, \tag{32}$$

where $x=\|\mathbf{x}\|, a>0, A>0, B>0, \alpha>0, \beta>0$,

$$C_T(a,t) = e^{-at}, \quad \mu(a) = e^{-a}.$$

It has been shown (Posa 2021) that (32) is an isotropic covariance function which always assumes negative values in a subset of its domain if and only if: $1<\frac{\alpha}{\beta}<\frac{A}{B}$.

If these last conditions on the parameters are satisfied, then the following covariance function

$$C(x,t,A,B,\alpha,\beta) = \int_0^\infty C_S(x;a,A,B,\alpha,\beta)C_T(a,t)\mu(a)da \tag{33}$$

is always positive in its domain.

Proof (See the Appendix). □

Corollary 5 *Let*

$$C_S(x;a) = e^{-ax}, \quad C_T(t,a) = \cos(a|t|), \quad \mu(a) = e^{-a}, x=\|\mathbf{x}\| \quad a>0,$$

then, the following space-time covariance function

$$C(x,t) = \int_0^\infty C_S(x;a)C_T(t,a)\mu(a)da = \frac{x+1}{(x+1)^2+t^2}, \tag{34}$$

is always positive in its domain.

Note that in the previous Corollary, the covariance function $C^*(x, t, a) = C_S(x; a)C_T(t, a)$ is separable, it is not strictly positive definite (De Iaco and Posa 2018) because the cosine covariance function is only positive definite and it can assume negative values in a subset of its domain; however, the integrated product (34) is non separable and it is strictly positive definite, moreover it is always positive.

Corollary 6 *Let*

$$C_S(x; a, A, B, \alpha, \beta) = Ae^{-a\alpha x} - Be^{-a\beta x}, \quad (35)$$

with $x = \|\mathbf{x}\|, a > 0, A > 0, B > 0, \alpha > 0, \beta > 0,$

$$C_T(a, t) = \cos\left(a|t|\right), \quad \mu(a) = e^{-a}.$$

It has been shown (Posa 2021) that (35) is an isotropic covariance function which always assumes negative values in a subset of its domain if and only if: $1 < \frac{\alpha}{\beta} < \frac{A}{B}$.

If these last conditions on the parameters are satisfied, then the following covariance function

$$C(x, t, A, B, \alpha, \beta) = \int_0^\infty C_S(x; a, A, B, \alpha, \beta), C_T(a, t)\mu(a)da \quad (36)$$

is always positive in its domain.

Proof (See the Appendix). □

Note that in the previous Corollary, the covariance function $C^*(x, t, a) = C_S(x; a)C_T(t, a)$ is separable, it is not strictly positive definite (De Iaco and Posa 2018) because the cosine covariance function is only positive definite and it can assume negative values in a subset of its domain; however, the integrated product (34) is non separable and it is strictly positive definite, moreover it is always positive.

Remarks

- According to Corollaries 4, 5, and 6, integrated product models could be always positive even if the basic models C_S and C_T are negative in a subset of their domain, hence they are not suitable to generate space-time covariance functions which can assume negative values in a subset of their domain.
- On the basis of the previous item, Cressie–Huang models are special cases of the integrated product models, hence they could be always positive on their spatial-temporal domain. In particular, the space-time covariance function in the example 4. of their paper (Cressie and Huang 1999) corresponds to the covariance function of Eq. (14) in De Iaco et al. (2002).
- Taking into account the prevoius items and the further result which claims that Gneiting models are always positive by constructions, the only models suitable to generate space-time covariance functions which can assume negative values in a subset of their domain are the product, the product sum, together with the modified versions, as well as Rodrigues and Diggle models.
- The modified class of Rodrigues and Diggle models in (31) can be further generalized without assuming the integrability of the correlation functions $\rho_{S,i}$ and $\rho_{T,i}, i = 1, 2$. The hypothesis of integrability has been assumed by the same authors (Rodrigues and Diggle 2010). Hence, if the correlation functions $\rho_{S,i}$ and $\rho_{T,i}, i = 1, 2$ are not necessarily integrable, then the modified class of product-sum models can be considered special cases of the modified class of Rodrigues and Diggle models by selecting $\rho_{S,2} = 1$ or $\rho_{T,2} = 1$ in (31).

3.4 General definition of separability/non separability

As already pointed out, expression (1) cannot be utilized for continuous covariance functions which can assume negative values. Indeed, if the spatial and temporal marginals are continuous covariance functions characterized by negative values, there always exists at least one point for which the same marginals are zero. Hence, in order to provide a more general definition of separability, expression (1) will be replaced by the indexes d and d' defined by expressions (2) or (3). In the following, a general definition of separability/non separability will be given, valid for any covariance function.

Definition 2 Let $C(\mathbf{x}, t, \boldsymbol{\Theta})$, $(\mathbf{x}, t) \in A \subseteq \mathbb{R}^n \times \mathbb{R}$, be a continuous covariance function of a second order stationary space-time random field, where $\boldsymbol{\Theta}$ is a vector of parameters; then the covariance function C is *separable* in the subset A if:

$$d(\mathbf{x}, t; \boldsymbol{\Theta}) = d'(\mathbf{x}, t; \boldsymbol{\Theta}) = 0, \qquad \forall\, (\mathbf{x}, t) \in A, \quad \forall\, \boldsymbol{\Theta}, \quad (37)$$

where d and d' have been defined in (2) and (3), respectively and the measure μ of the set A satisfies the condition $\mu(A) > 0$; on the other hand, the covariance function C is non separable in the subset A if:

$$\begin{aligned} &d(\mathbf{x}, t; \boldsymbol{\Theta}) \neq 0 \qquad \forall\, (\mathbf{x}, t) \in B \subseteq A; \\ &d(\mathbf{x}, t; \boldsymbol{\Theta}) = 0, \quad \forall\, (\mathbf{x}, t) \in A - B, \end{aligned} \quad (38)$$

where the measure μ of the set B satisfies the condition $\mu(B) > 0$ and $\mu(A - B) = 0$.

Moreover, the covariance function C is uniformly positive *non separable* in the subset A if:

$$d(\mathbf{x},t;\mathbf{\Theta})>0 \ and \ d'(\mathbf{x},t;\mathbf{\Theta})>0 \quad \forall(\mathbf{x},t)\in A, \tag{39}$$

where: $C(\mathbf{x},t,\mathbf{\Theta})>0\ \forall(\mathbf{x},t)\in A,\forall\mathbf{\Theta}$, and the measure μ of the set A satisfies the condition $\mu(A)>0$; alternatively, the covariance function C is uniformly negative *non separable* in the subset A if:

$$d(\mathbf{x},t;\mathbf{\Theta})<0 \quad and \quad d'(\mathbf{x},t;\mathbf{\Theta})<0 \qquad \forall(\mathbf{x},t)\in A, \tag{40}$$

where: $C(\mathbf{x},t,\mathbf{\Theta})>0 \quad \forall(\mathbf{x},t)\in A,\forall\mathbf{\Theta}$, and the measure μ of the set A satisfies the condition $\mu(A)>0$.

According to the above Definition, the following result can be established.

Corollary 7 *A space-time correlation function ρ is separable in a subset A if and only if*

$$\rho(\mathbf{x},t)=\rho_S(\mathbf{x})\rho_T(t), \qquad \forall(\mathbf{x},t)\in A,$$

and the measure μ of the set A satisfies the condition $\mu(A)>0$.

Taking into account the previous Corollary, the only separable space-time covariance model is the product model.

Remarks

- Note that Definition 1 is a special case of Definition 2; in particular, if a spatio-temporal correlation function is always positive, together with its marginals, Definition 1 gets back; in particular, Definition 2 is valid for any spatio-temporal covariance function, even if it assumes negative values, although the concepts of uniformly positive and negative non separability can be given just for positive covariance functions;
- according to the previous item, as will be shown in the next Section, the space-time correlation models (47) and (48) assume negative values and they are non separable in the subset $A=[(0,+\infty)\times(0,+\infty)]$, hence $d(\mathbf{x},t;\mathbf{\Theta})\neq 0\,\forall(\mathbf{x},t)\in B\subset A$; the measure of B is positive and $d(\mathbf{x},t;\mathbf{\Theta})=0\,\forall(\mathbf{x},t)\in A-B$, however the measure of this last set is zero;
- according to the revised Definition 2, the concept of separability/non separability is related to the subset of the spatio-temporal domain of the covariance function. For example, a space-time covariance function can be separable in a certain subset and non separable in a different subset of its domain, as shown hereafter. Consider the following space-time correlation model:

$$\begin{aligned}&\rho(x,t)=k_1 Sph(x;a_1)Sph(t;a_2)+k_2 Sph(x;a_3),\\&k_1>0,k_2>0,k_1+k_2=1,\end{aligned} \tag{41}$$

  where $x=\|\mathbf{x}\|$ and:

$$Sph(r;a)=\begin{cases}1-\dfrac{3r}{2a}+\dfrac{1}{2}\left(\dfrac{r}{a}\right)^3 & r\leq a\\ 0 & r>a,\end{cases} \tag{42}$$

  is the spherical correlation model, moreover $0<a_3<a_1,a_2>0$. It is trivial to check that model (41) is non separable in the subset $A=[(0,a_3)\times(0,a_2)]$ and it is separable in the subset $C=[(a_3,a_1)\times(0,+\infty)]$ and the measures of the sets A and C are different from zero;
- note that the index d (or d') does not depend on the peculiar correlation model for what concerns the classes of the sum model, the product sum model and Gneiting family: infact the index d (or d') is always negative for the sum and product sum models and it is always positive for the Gneiting family, indipendently from the correlation functions utilized. Moreover, for the sum and product sum models, the index d (or d') is always negative even if the correlation functions are negative;
- on the other hand, for what concerns the integrated product and product-sum, Cressie, Rodrigues and Diggle families and the modified product-sum models, the sign of the index d (or d') strongly depends on the correlation functions utilized: indeed, these last models are able to describe any kind of non separability.

4 Graphical representation of the results

In the present Section graphical representations of some classes of space-time correlation functions, described in the previous Section, will be provided. In particular, it will be shown how these wider classes of correlation functions are able to describe positive and negative correlations by suitably modifying the parameters values on which the same classes depend.

4.1 Separable space-time isotropic correlation functions

Flexible classes of separable space-time correlation functions, characterized by positive and negative values and by various behaviour near the origin, can be suitably obtained by using some relevant results concerning the difference between covariance functions, given in Posa (2021) and utilizing Theorem 1. Among the various results, it has been shown that the following isotropic correlation class:

$$\begin{aligned}\rho(s;A,B,\alpha,\beta)&=A\exp(-\alpha s)-B\exp(-\beta s),\\&A>0,B>0,\quad A-B=1,\end{aligned} \tag{43}$$

is capable to describe several behaviours: models which are always positive, as well as models which are characterized

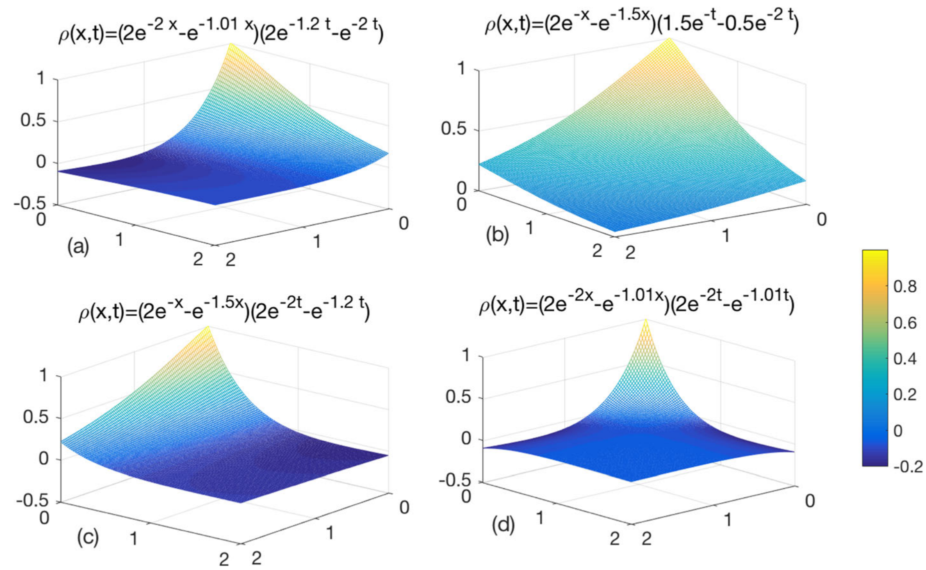

Fig. 2 Behaviour of model (44) where both marginals present a linear behaviour near the origin. In **a** the spatial marginal is negative in a subset of its domain, whereas the temporal marginal is always positive; in **b** both marginals are always positive; in **c** the spatial marginal is always positive, whereas the temporal marginal is negative in a subset of its domain; in **d** both marginals are negative in a subset of their domain

by negative values, in addition to models which present a linear or a parabolic behaviour in proximity of the origin. Moreover, according to the values of parameters on which this family depends, there could be an inflection point, such that the concavity is downwards in proximity of the origin: this last behaviour is atypical for covariance functions characterized by a linear behaviour near the origin.

In particular, (43) is a correlation function if and only if:

$1 < \frac{\beta}{\alpha} \le \frac{A}{B}, \quad or \quad 1 < \frac{\alpha}{\beta} < \frac{A}{B}.$

If $1 < \frac{\beta}{\alpha} < \frac{A}{B}$ or $1 < \frac{\alpha}{\beta} < \frac{A}{B}$, then the correlation function (43) always presents a linear behaviour near the the origin. If $1 < \frac{\beta}{\alpha} = \frac{A}{B}$, the correlation function (43) presents a parabolic behavior near the origin; moreover, if $1 < \frac{\alpha}{\beta} < \frac{A}{B}$, the correlation function (43) is always negative in a subset of its field of definition. At last, if $1 < \frac{\beta}{\alpha} \le \frac{A}{B}$, the correlation function (43) cannot ever be negative.

According to the previous results, the following separable class of space-time isotropic correlation functions:

$$\rho(x, t, \mathbf{\Theta}) = (A_1 e^{-\alpha_1 x} - B_1 e^{-\beta_1 x})(A_2 e^{-\alpha_2 t} - B_2 e^{-\beta_2 t}), \qquad (44)$$

where $A_i > 0, B_i > 0, \quad A_i - B_i = 1, i = 1, 2, \mathbf{\Theta} = (\alpha_1, \beta_1, \alpha_2, \beta_2, A_1, B_1, A_2, B_2)$, can handle situations for which both marginals are characterized by a linear behaviour near the origin, together with various combinations for which both marginals are characterized by positive or negative values, by suitably changing the values of the parameters vector $\mathbf{\Theta}$, as previously described. In particular, in Fig. 2a the spatial marginal assumes negative values in a subset of its domain, whereas the temporal marginal is always positive; in Fig. 2b both marginals always assume positive values, whereas in Fig. 2c the spatial marginal is always positive and the temporal marginal assumes negative values in a subset of its domain; at last, in Fig. 2d both marginals assume negative values in a subset of their domain. Note that both marginals in Fig. 2a–d present a linear behaviour near the origin. Moreover, the expression of the correlation functions utilized in each of the above figures, is represented on the top of the same figures.

On the basis of the results given in Posa (2021), the family of correlation functions

$$\rho(x; A, B, \alpha, \beta) = Ae^{-\alpha x^2} - Be^{-\beta x^2}, \quad A > 0, B > 0, A - B = 1, \qquad (45)$$

is an isotropic correlation function in $\mathbb{R}^2$ if and only if:

$$1 < \frac{\alpha}{\beta} < \frac{A}{B}. \qquad (46)$$

The class (45) is extremely flexible to describe some peculiar behaviours of correlation structures: infact, this class, according to the values of the parameters, i.e. $1 < \frac{\alpha}{\beta} < \frac{A}{B}$, always assumes a parabolic behaviour in proximity of the origin, moreover, the same class is always negative in a subset of its domain.

Hence, in order to describe separable space-time correlation models for which both marginals are characterized by a parabolic behaviour near the origin (Fig. 3), the classes (21), (43) and (45) can be suitably combined according to the required behaviour. As already pointed out, the class (43) presents a parabolic behaviour near the origin if $1 < \frac{\beta}{\alpha} = \frac{A}{B}$ and it is always positive; the class (45)

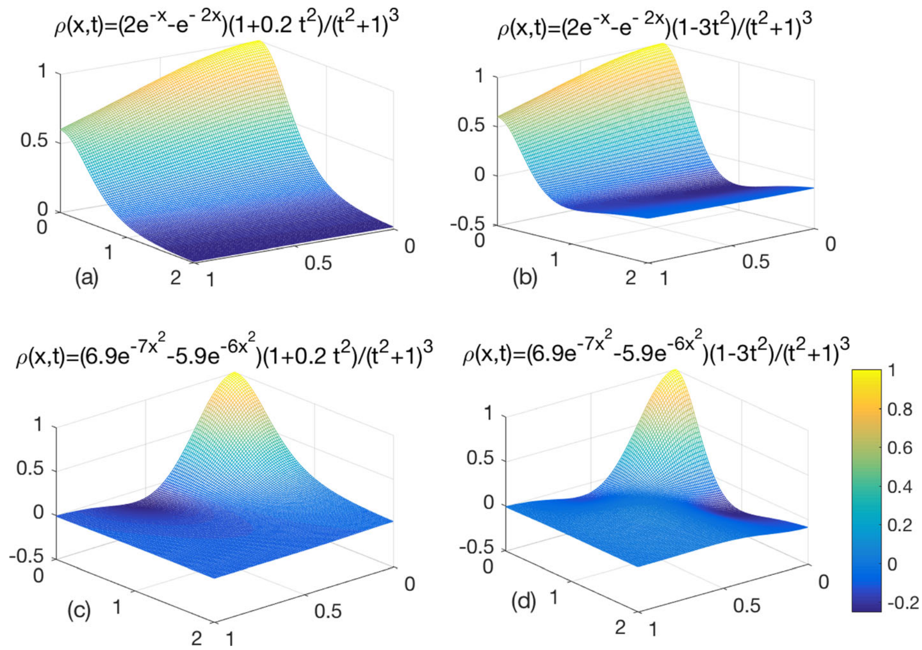

Fig. 3 The classes (21), (43) and (45) are suitably combined so that both marginals present a parabolic behaviour near the origin. In **a** both marginals always assume positive values; in **b** the spatial marginal is always positive, whereas the temporal marginal is negative in a subset of its domain; in **c** the spatial marginal is negative in a subset of its domain, whereas the temporal marginal is always positive; in **d** both marginals are negative in a subset of their domain

always presents a parabolic behaviour near the origin and it is always negative in a subset of its domain, whereas the class (21) always presents a parabolic behaviour near the origin and can assume always positive values, as well as negative values in a subset of its domain, according to the value of the parameter k. In Fig. 3a both marginals always assume positive values; in Fig. 3b the spatial marginal is always positive and the temporal marginal assumes negative values in a subset of its domain; viceversa, in Fig. 3c the spatial marginal assumes negative values in a subset of its domain, whereas the temporal marginal is always positive; at last, in Fig. 3d both marginals assume negative values in a subset of their domain. Note that both marginals in Fig. 3a–d present a parabolic behaviour near the origin. Moreover, the expression of the correlation functions utilized in each of the above figures, is represented on the top of the same figures.

Putting together all the previous results, separable models characterized by a parabolic behaviour near the origin for the spatial marginal and a linear behaviour near the origin for the temporal marginal, can be obtained, as shown in Fig. 4. In Fig. 4a both marginals always assume positive values; in Fig. 4b the spatial marginal is always positive and the temporal marginal assumes negative values in a subset of its domain; viceversa, in Fig. 4c the spatial marginal assumes negative values in a subset of its domain, whereas the temporal marginal is always positive; at last, in Fig. 4d both marginals assume negative values in a subset of their domain. Moreover, the expression of the correlation functions utilized in each of the above figures, is represented on the top of the same figures.

4.2 Non separable space-time isotropic correlation functions

As already undelined in the previous Sect. 3, considering the various classes of non separable correlation functions, the modified product-sum models and the modified version of Rodrigues and Diggle models can be considered among the most flexible to describe non separable space-time correlation functions characterized by positive and negative values.

Some peculiar graphical representations for the class of models (27), (28) and (31) is given hereafter. In particular, for the following non separable space-time class of modified product-sum models:

$$\rho(x,t,A,B) = A\left(6.9e^{-7x^2} - 5.9e^{-6x^2}\right)\frac{1-3t^2}{(t^2+1)^3} + B\frac{1-3x^2}{(x^2+1)^3}, \tag{47}$$

the spatial and temporal marginals always present a parabolic behaviour near the origin; moreover:

$$\lim_{x\to\infty}\rho(x,t) = 0; \qquad \lim_{t\to\infty}\rho(x,t) = B\frac{1-3x^2}{(x^2+1)^3}.$$

According to the previous results, the space-time correlation model always goes to zero along the spatial axis, whereas it reaches a limit value along the temporal axis which depends on x and on the parameter B. In Fig. 5 it is shown the bahaviour of model (47) for different values of the parameters A and B, whose values are represented at the top of each figure. Note that the spatial marginal is always

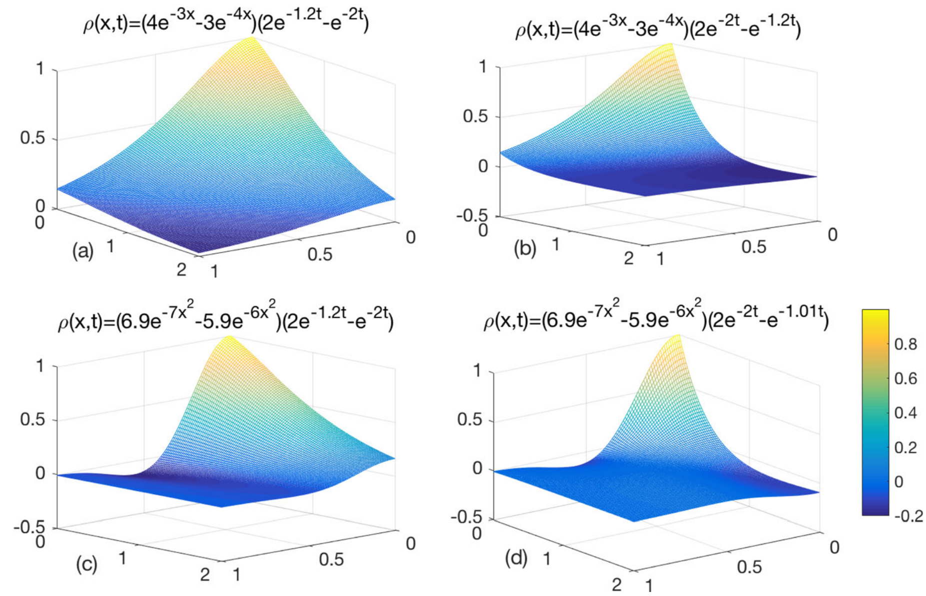

Fig. 4 The classes (43) and (45) are suitably combined so that the spatial marginal presents a parabolic behaviour near the origin, whereas the temporal marginal presents a linear behaviour near the origin. In **a** both marginals always assume positive values; in **b** the spatial marginal is always positive, whereas the temporal marginal is negative in a subset of its domain; in **c** the spatial marginal is negative in a subset of its domain, whereas the temporal marginal is always positive; in **d** both marginals are negative in a subset of their domain

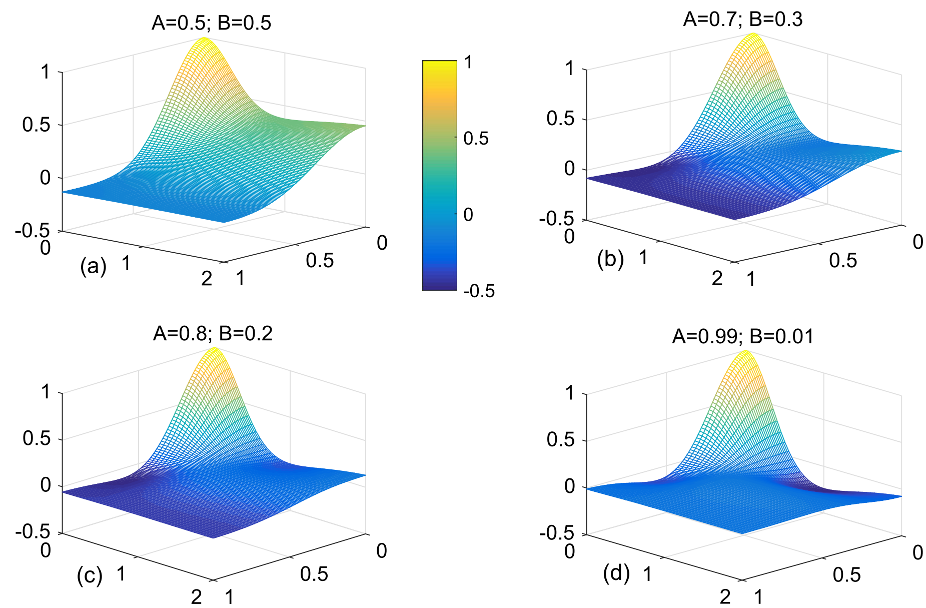

Fig. 5 Bahaviour of the non separable model (47) for different values of the parameters A and B, whose values are represented at the top of each figure. The spatial marginal is always negative in a subset of its domain, whereas the behaviour of the temporal marginal depends on the value of the parameter B: as B goes to zero, the temporal marginal assumes negative values and the above model is very close to a separable model

negative in a subset of its domain, whereas the behaviour of the temporal marginal depends on the value of the parameter B. As B goes to zero, the temporal marginal assumes negative values and the above model is very close to a separable model: in this case, model (47) can be considered as nuisance to a separable model.

On the other hand, for the following non separable space-time class of modified product-sum models:

$$\begin{aligned}\rho(x,t,A,B) =& A(6.9e^{-7x^2} - 5.9e^{-6x^2})\frac{1-3t^2}{(t^2+1)^3} \\ &+ B\frac{1-t^2}{(t^2+1)^3},\end{aligned} \tag{48}$$

although the spatial and temporal marginals always present a parabolic behaviour near the origin, however:

$$\lim_{x\to\infty}\rho(x,t) = B\frac{1-t^2}{(t^2+1)^3}; \qquad \lim_{t\to\infty}\rho(x,t) = 0.$$

According to the previous results, the space-time correlation model always goes to zero along the temporal axis, whereas it reaches a limit value along the spatial axis which depends on t and on the parameter B. In Fig. 6 it is shown the bahaviour of model (48) for different values of the parameters A and B, whose values are represented at the top of each figure. Note that the temporal marginal is always negative in a subset of its domain, whereas the behaviour of the spatial marginal depends on the value of

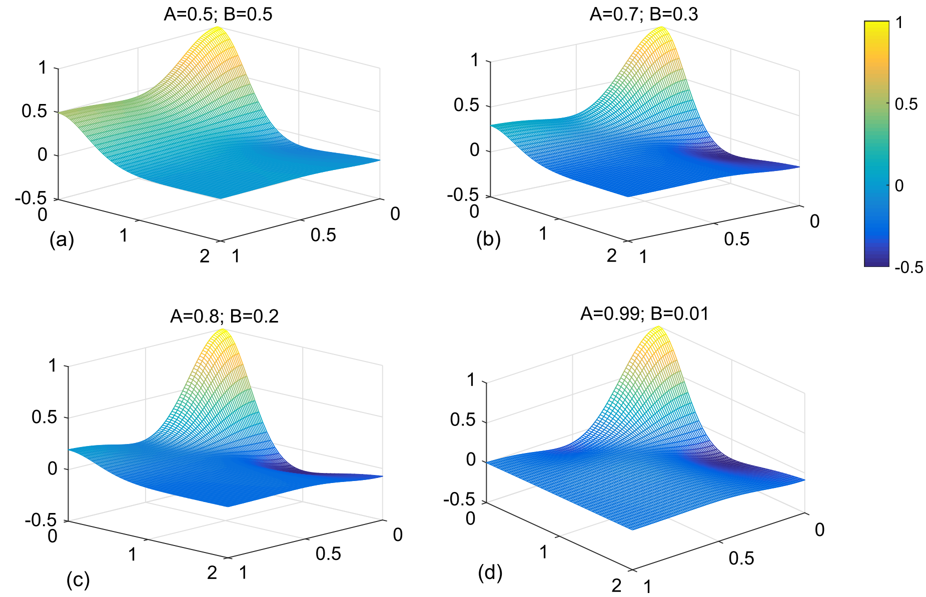

Fig. 6 Bahaviour of the non separable model (48) for different values of the parameters A and B, whose values are represented at the top of each figure. Note that the temporal marginal is always negative in a subset of its domain, whereas the behaviour of the spatial marginal depends on the value of the parameter B. As B goes to zero, the spatial marginal assumes negative values and the above model is very close to a separable model

the parameter B. As B goes to zero, the spatial marginal assumes negative values and the above model is very close to a separable model: in this case, model (48) can be considered as nuisance to a separable model.

In the following some non separable space-time isotropic models belonging to the modified class of Rodrigues and Diggle models given in (31) will be analyzed. In particular, for the family defined hereafter:

$$\rho(x,t,A,B) = A\left(6.9e^{-7x^2} - 5.9e^{-6x^2}\right)\frac{1-3t^2}{(t^2+1)^3} + B(5e^{-7x^2} - 4e^{-6x^2})e^{-t}, A>0, B>0, \tag{49}$$

$\lim_{x\to\infty}\rho(x,t) = \lim_{t\to\infty}\rho(x,t) = \lim_{\|(x,t)\|\to\infty}\rho(x,t) = 0$, moreover, the spatial marginal always presents a parabolic behaviour near the origin and always assumes negative values in a subset of its domain. On the other hand, the temporal marginal always presents a linear behaviour near the origin; indeed, according to the values of parameters on which this family depends, there could be an inflection point, such that the concavity is downwards in proximity of the origin: this last behaviour is atypical for covariance functions characterized by a linear behaviour near the origin (Posa 2023). Moreover, the temporal marginal can always assume positive values, as well as negative values in a subset of its domain by suitably varying the values of the parameter B, which could be considered a nuisance parameter; in fact, as B goes to zero, model (49) becomes very close to a separable correlation function. In Fig. 7 it is shown the bahaviour of model (49) for different values of the parameters A and B, whose values are represented at the top of each figure. For the following family,

$$\rho(x,t,A,B) = Ae^{-x}\frac{1-3t^2}{(t^2+1)^3} + B(5e^{-7x^2} - 4e^{-6x^2})\frac{1-2t^2}{(t^2+1)^3}, \quad A>0, B>0, \tag{50}$$

$\lim_{x\to\infty}\rho(x,t) = \lim_{t\to\infty}\rho(x,t) = \lim_{\|(x,t)\|\to\infty}\rho(x,t) = 0$, moreover the temporal marginal always presents a parabolic behaviour near the origin and always assumes negative values in a subset of its domain. On the other hand, the spatial marginal always presents a linear behaviour near the origin: indeed, as in the previous case, according to the values of parameters on which this family depends, there could be an inflection point, such that the concavity is downwards in proximity of the origin. Moreover, the spatial marginal can always assume positive values, as well as negative values in a subset of its domain by suitably varying the values of the parameter B, which could be considered a nuisance parameter; in fact, as B goes to zero, model (50) becomes very close to a separable correlation function. In Fig. 8 it is shown the bahaviour of model (50) for different values of the parameters A and B, whose values are represented at the top of each figure. For the family defined hereafter,

$$\rho(x,t,A,B) = Ae^{-x}\frac{1-3t^2}{(t^2+1)^3} + Be^{-3x}\frac{1-2t^2}{(t^2+1)^3}, \quad A>0, B>0, \tag{51}$$

$\lim_{x\to\infty}\rho(x,t) = \lim_{t\to\infty}\rho(x,t) = \lim_{\|(x,t)\|\to\infty}\rho(x,t) = 0$, moreover the temporal marginal always presents a parabolic behaviour near the origin and always assumes negative values

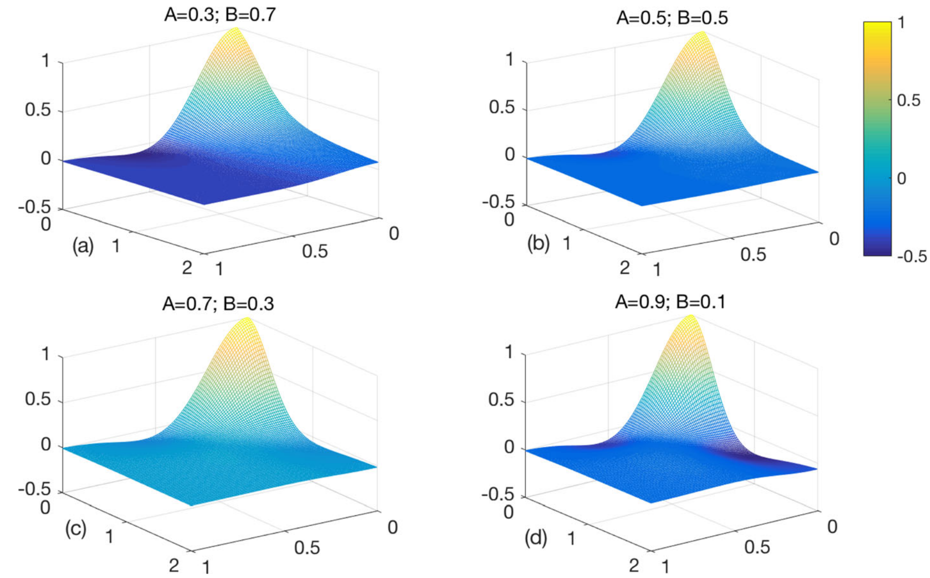

Fig. 7 Bahaviour of the non separable model (49) for different values of the parameters A and B, whose values are represented at the top of each figure. The spatial marginal always presents a parabolic behaviour near the origin and always assumes negative values in a subset of its domain. On the other hand, the temporal marginal always presents a linear behaviour near the origin: indeed, according to the values of parameters on which this family depends, there could be an inflection point, such that the concavity is downwards in proximity of the origin: this last behaviour is atypical for covariance functions characterized by a linear behaviour near the origin. Moreover, the temporal marginal can always assume positive values, as well as negative values in a subset of its domain by suitably varying the values of the parameter B, which could be considered a nuisance parameter; in fact, as B goes to zero, model (49) becomes very close to a separable correlation function

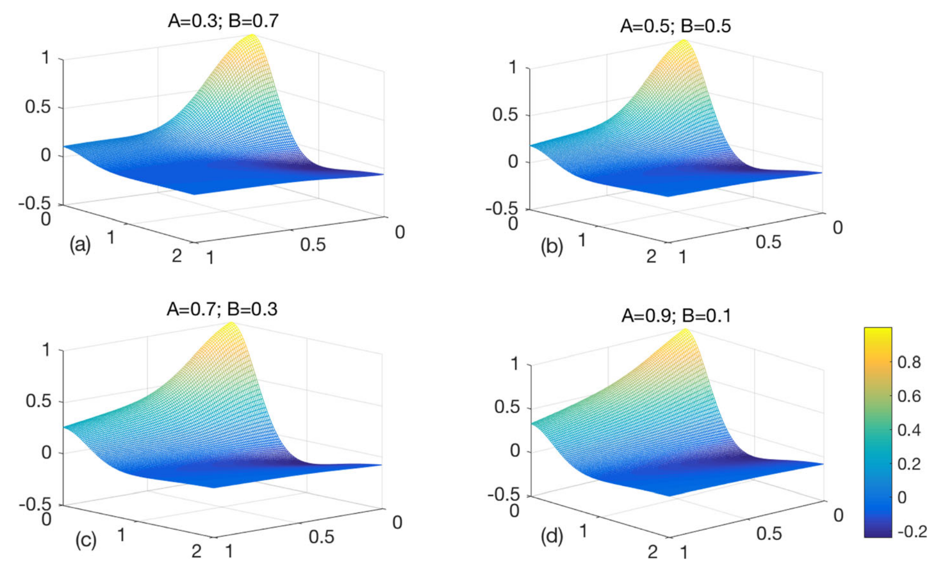

Fig. 8 Bahaviour of the non separable model (50) for different values of the parameters A and B, whose values are represented at the top of each figure. The spatial marginal always presents a linear behaviour near the origin: indeed, according to the values of parameters on which this family depends, there could be an inflection point, such that the concavity is downwards in proximity of the origin. Moreover, the spatial marginal can always assume positive values, as well as negative values in a subset of its domain by suitably varying the values of the parameter B, which could be considered a nuisance parameter; in fact, as B goes to zero, model (50) becomes very close to a separable correlation function

in a subset of its domain. On the other hand, the spatial marginal always presents a linear behaviour near the origin; moreover, the spatial marginal always assumes positive values. As the parameter B goes to zero, model (51) becomes very close to a separable correlation function. In Fig. 9 it is shown the bahaviour of model (51) for different values of the parameters A and B, whose values are represented at the top of each figure. For the following family,

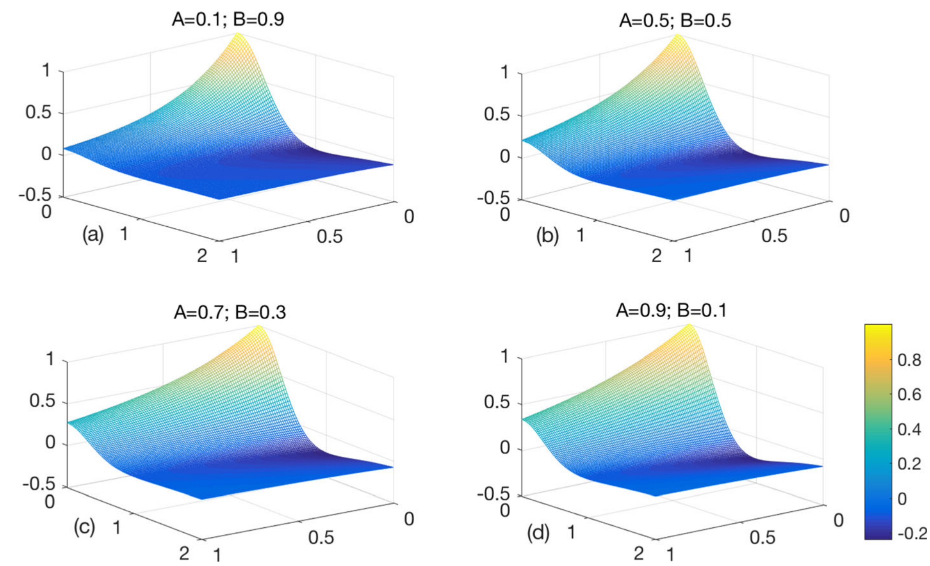

Fig. 9 Bahaviour of the non separable model (51) for different values of the parameters A and B, whose values are represented at the top of each figure. The temporal marginal always presents a parabolic behaviour near the origin and always assumes negative values in a subset of its domain. On the other hand, the spatial marginal always presents a linear behaviour near the origin; moreover, the spatial marginal always assumes positive values. As the parameter B goes to zero, model (51) becomes very close to a separable correlation function

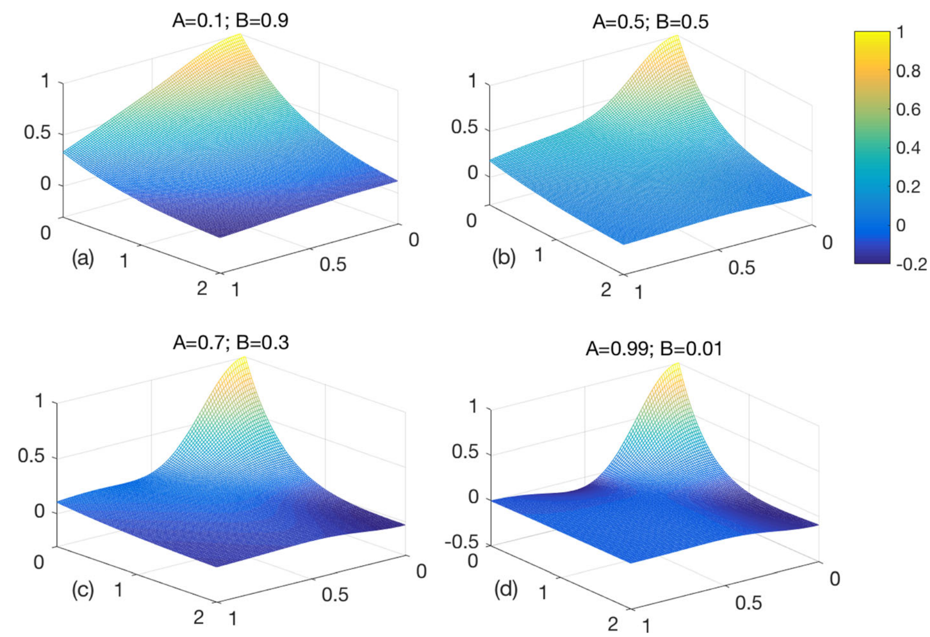

Fig. 10 Bahaviour of the non separable model (52) for different values of the parameters A and B, whose values are represented at the top of each figure. The spatial marginal always presents a parabolic behaviour near the origin and it always assumes positive values for the values of the parameter $B > 0.2$, as it is shown in (**a**), (**b**) and (**c**). On the other hand, the temporal marginal always presents a linear behaviour near the origin, moreover the temporal marginal always assumes positive values for values of the parameter $B > 0.3$. Note that both marginals assume negative values in a subset of their domain if the parameter B is very close to zero; in particular, in this last case, model (52) becomes very close to a separable correlation function and the parameter B can be considered a nuisance parameter

$$\rho(x,t,A,B) = A\left(6.9e^{-7x^2} - 5.9e^{-6x^2}\right)\left(2e^{-2t} - e^{-1.01t}\right) + Be^{-x^2}e^{-t}, A > 0, B > 0, \tag{52}$$

$\lim_{x\to\infty}\rho(x,t) = \lim_{t\to\infty}\rho(x,t) = \lim_{\|(x,t)\|\to\infty}\rho(x,t) = 0$, moreover the spatial marginal always presents a parabolic behaviour near the origin and it always assumes positive values for the values of the parameter $B > 0.2$, as it is shown in Fig. 10a–c. On the other hand, the temporal marginal always presents a linear behaviour near the origin, moreover the temporal marginal always assumes positive values for values of the parameter $B > 0.3$. Note that both marginals assume negative values in a subset of their domain if the parameter B is very close to zero; in particular, in this last case, model (52) becomes very close to a separable correlation function and the parameter B can be considered a nuisance parameter. In Fig. 10 it is shown the bahaviour of model (52) for different values of the parameters A and B, whose values are represented at the top of each figure.

4.2.1 A general class of space-time correlation functions

A general and wide description of several classes of space-time correlation functions has been provided in this paper, analyzing some merits and drawbacks of the same classes. By utilizying and putting together all the previous results, the following general class of space-time correlation functions has been proposed:

$$\rho(\mathbf{x},t;\boldsymbol{\Theta}) = A\rho_{S,1}(\mathbf{x};\theta_1)\rho_{T,1}(t;\phi_1) + B\rho_{S,2}(\mathbf{x};\theta_2)\rho_{T,2}(t;\phi_2), A>0, B>0, A+B=1, \tag{53}$$

where $\boldsymbol{\Theta} = (A, B, \theta_1, \phi_1, \theta_2, \phi_2)$ and $\rho_{S,1}(\mathbf{x};\theta_1), \rho_{S,2}(\mathbf{x};\theta_2), \rho_{T,1}(t;\phi_1), \rho_{T,2}(t;\phi_2)$ are, respectively, two valid and not necessarily integrable spatial and two valid and not necessarily integrable temporal correlation functions, not necessarily constrained to be positive; hence the non separable space-time correlation function ρ and the marginal correlations can assume positive or negative values by properly choosing the parameters values of the correlation functions $\rho_{S,\cdot}$ and $\rho_{T,\cdot}$ as in (22) and in (23) and the weights A and B.

The class (53) is characterized by an extremely simple formalism and can be easily adapted to several case studies, as shown through the graphical representation in the previous Section. Indeed modelling and computational advantages of this class can be easily summarized as follows:

- if all the correlation functions in (53) are integrable and $A = B$, then the classical Rodrigues and Diggle class is obtained;
- if $B = 0$ then the class (53) is separable; as already underlined, classes of separable space-time correlation functions, characterized by positive and negative values and by various behaviour near the origin, can be suitably obtained by using some relevant results concerning the difference between covariance functions, given in Posa (2021) and utilizing Theorem 1 (see Figs.2,3 and 4);
- if $\rho_{S,2} = 1$ or $\rho_{T,2} = 1$ in (53), then the modified product-sum models (28) and (27), respectively, can be obtained; these last classes of models are particularly useful to describe correlation structures which do not decay asymptotically to zero along space or time (see Figs. 5 and 6);
- as previously underlined, the class (53) is flexible enough to describe positive and negative correlation structures, as well as various behaviours near the origin, according to the choice of the correlation functions involved and to the values of the parameters. In particular, negative spatial correlation refers to phenomena where the values of a variable tend to be dissimilar when they are geographically proximate; this situation is consistent with the wave-hole semivariogram model specification, which resembles a second-order temporal autoregressive structure having first-order positive and second-order negative autocorrelation. By nature, negative spatial correlation materializes with a spatial competitive process. For example, it has been discovered in forest competition for light (Montgomery and Chazdon 2001), in the geographic distribution of lung cancer rates (Hu et al. 2018) and in georeferenced data (Jacob et al. 2011). Furthermore, Gray and Shadbegian (2007) detect weak negative spatial correlation in 102 industrial plant emissions of sulfur dioxide and nitrogen oxides across the medium-size United States cities;
- various asymptotic behaviours along space and time can be described through the class of models (53): in particular, if all the correlation functions involved in (53) are integrable, then the same class decays asymptotically to zero along any spatial-temporal direction, in particular along space and time separately. Moreover, if one or more than one of the correlation functions involved in (53) is not integrable, then the class of models (53) does not decay asymptotically to zero along space or time;
- if all the correlation functions involved in (53) are positive, then the same class of models can describe any kind of separability.

4.2.2 Computational aspects

The choice of an appropriate model within the class (53) can be supported by analyzing some main properties, such as separability/non-separability, type of non-separability (if the correlation model is assumed to be positive) and behaviour near the origin of the spatio-temporal sample correlation function; the related computational aspects were developed in Cappello et al. (2020) and some statistical tests can be used for this purpose (Cappello et al. 2018).

Regarding parameters estimation, as a starting point, it is necessary to compute the sample correlation function $\widehat{\rho}$. Given the set $A = \{(\mathbf{s}_i, t_i), i = 1, 2 \ldots, n\}$ of data locations in space-time, where

$$L(\mathbf{r}_s, r_t) = \{(\mathbf{s}+\mathbf{h}_s, t+h_t) \in A, (\mathbf{s}, t) \in A : \mathbf{h}_s \in Tol(\mathbf{r}_s) \text{ and } h_t \in Tol(r_t)\},$$

and $Tol(\mathbf{r}_s)$, $Tol(r_t)$ are, respectively, some specified tolerance regions around $\mathbf{r}_s$ and r_t and $|L(\mathbf{r}_s, r_t)|$ is the cardinality of the set $L(\mathbf{r}_s, r_t)$, a suitable class of correlation functions $\rho(\cdot, \boldsymbol{\Theta})$ belonging to (53), which depends on a vector of parameters $\boldsymbol{\Theta}$, must be fitted to the empirical correlation $\widehat{\rho}$, as usually done. In particular, the vector of parameters $\boldsymbol{\Theta}$ can be estimated through the non-linear weighted least squares technique, by minimizing the following function:

$$\Psi(\boldsymbol{\Theta}) = \sum_{i=1}^{n} \left[\widehat{\rho}(\mathbf{s}_i, t_i) - \rho(\mathbf{s}_i, t_i; \boldsymbol{\Theta})\right]^2 w_i,$$

where w_i represents the weight of the i-th lag. These weights are reasonably assumed to be equal to the number of pairs related to the same lag.

After modeling the space-time empirical correlation, the subsequent step is to evaluate the reliability of the fitted model through the application of spatio-temporal cross-validation and jackknife techniques.

5 Conclusions

In this paper some traditional families of space-time covariance functions, proposed in the literature, have been properly reviewed in order to enrich the same families with models characterized by negative values in a subset of their domain. Furthermore, the definition of separability has been revised in order to enlarge the classical definition. These new families of covariances present flexible and interesting features with respect to most of the classical families of isotropic covariance models. Indeed, as it has been underlined throughout the paper, the Whittle–Matern family and the whole classes of models obtained by applying the usual properties of the covariance functions, are not able to describe correlation structures which present negative values. From a practical point of view, these new classes of isotropic covariance models are characterized by an extremely simple formalism and can be easily adapted to several case studies.

Appendix

Proof of Corollary 1 According to definition (3), if $C_S(\mathbf{x}) > 0 \quad \forall \mathbf{x}$ and $C_T(t) > 0 \quad \forall t$:

$$\begin{aligned} d'(\mathbf{x}, t) &= C(\mathbf{x}, t)C(\mathbf{0}, 0) - C(\mathbf{x}, 0)C(\mathbf{0}, t) = \\ &= \left[C_S(\mathbf{x}) + C_T(t)\right]\left[C_S(\mathbf{0}) + C_T(0)\right] \\ &\quad - \left[C_S(\mathbf{x}) + C_T(0)\right]\left[C_S(\mathbf{0}) + C_T(t)\right] = \\ &= -\left[C_S(\mathbf{0}) - C_S(\mathbf{x})\right]\left[C_T(0) - C_T(t)\right] < 0, \end{aligned} \tag{54}$$

taking into account one of the main properties of a covariance function: $C_S(\mathbf{0}) \geq |C_S(\mathbf{x})|$ and $C_T(0) \geq |C_T(t)|$. Indeed, under the hypothesis of second order stationarity, the above index can be equivalently written as follows: $d'(\mathbf{x}, t) = -\gamma_S(\mathbf{x})\gamma_T(t)$, where γ_S and $\gamma_T(t)$ are the spatial marginal and temporal marginal semivariogram, respectively. □

Proof of Theorem 1 It is well known that (21) is a correlation function if and only if its Fourier transform:

$$f(\omega, k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \cos(\omega t) \frac{1 - kt^2}{(t^2 + 1)^3} dt,$$

is a spectral density function. Note that:

$$\begin{aligned} &\frac{1}{2\pi} \int_{-\infty}^{+\infty} \cos(\omega t) \frac{1 - kt^2}{(t^2 + 1)^3} dt \\ &\quad = \frac{e^{-|\omega|}}{16} \left[\omega^2(1 + k) + \omega(3 - k) + 3 - k\right], \end{aligned}$$

hence it is integrable and $f(\omega, k) \geq 0$ if and only if $-\frac{1}{5} \leq k \leq 3$. The class of parametric correlation functions (21) always presents a parabolic behaviuor in proximity of the origin, moreover it is flexible enough because it can model positive correlation structures as well as correlation structures which can assume negative values in a subset of their domain; indeed, according to the value of the parameter k, it can be always positive if $-\frac{1}{5} \leq k \leq 0$, and can assume negative values in a subset of its domain if $0 < k \leq 3$. For $t > 0$, $\rho(t_m) = \frac{-4k^3}{27(k+1)^2}$ is the minimum value assumed by (21), where $t_m = \sqrt{\frac{1}{2} + \frac{3}{2k}}$. As a consequence, as k increases, $\rho(t_m)$ becomes more and more negative; in particular, according to the results of Theorem 1, the lowest value of $\rho(t_m)$ is obtained for $k = 3$, i.e., $\rho(t_m) = -0.25$. □

Proof of Corollary 4 Note that

$$\begin{aligned} &\int_0^{\infty} C_S(x; a, A, B, \alpha, \beta) C_T(a, t) \mu(a) da \\ &\quad = \frac{x(A\beta - B\alpha) + t(A - B) + A - B}{(\alpha x + t + 1)(\beta x + t + 1)}, \end{aligned} \tag{55}$$

hence, taking into account the hypotheses on the parameters, i.e., $A\beta - B\alpha > 0, A - B > 0$, expression (55) is always positive. □

Proof of Corollary 6 Let: $A\beta - B\alpha = \delta_1 > 0$, $A\alpha - B\beta = \delta_2 > 0$, $A - B = \delta_3 > 0$, then:

$$\begin{aligned} &\int_0^{\infty} C_S(x; a, A, B, \alpha, \beta), C_T(a, t) \mu(a) da = \\ &= \frac{(\alpha\beta\delta_1 x^2 + \delta_2 t^2 + 2\delta_1 + \delta_2)x + [\delta_1(\alpha + \beta) + \alpha\beta\delta_3]x^2 + \delta_3(t^2 + 1)}{2(\alpha + \beta)(\alpha\beta x^2 + t^2 + 1)x + \alpha^2\beta^2 x^4 + [(\alpha^2 + \beta^2)t^2 + \alpha^2 + \beta^2 + 4\alpha\beta]x^2 + (t^2 + 1)^2}, \end{aligned} \tag{56}$$

hence taking into account the hypotheses on the parameters, expression (56) is always positive.

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Declarations

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