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Characteristics of some isotropic covariance models with negative values

De Iaco S. *, Posa D.

Department of Economic Sciences, University of Salento, Lecce, Italy

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ABSTRACT

In the literature, most of the classical covariance models characterised by negative values were derived by utilising the Bessel functions, on the other hand, recently, other classes of models with negative correlation were obtained through the difference between two covariance functions. However, although for the former, the analytic features, such as their absolute minimum values, were completely explored, for the latter these aspects have to be still investigated. In this paper, starting from the admissibility conditions and the general characteristics of three wide families of isotropic covariance models, based on the difference of Gaussian, exponential and rational models, their absolute minimum, as a function of the dimension of the Euclidean space in which they are defined, is provided. Consequently, the minimum values for the most common Euclidean dimensional spaces are given as special cases. These results fill the theoretical gap related to the analysed classes of correlation models with negative values and then can support their use. A simulation study and an application to a real data set are also presented to assess performance in terms of prediction accuracy.

1. Introduction

Correlation models with negative values are receiving a lot of attention from the scientific community, since they are required in many applications concerning phenomena related to turbulence in space or space–time, mining, geology and hydrology, as described by some authors, such as Yaglom (1955), Journel and Huijbregts (1981), Matérn (1980), Levinson et al. (1984), Yakhot et al. (1989), Shkarofsky (1968), Pomeroy et al. (2003), Xu et al. (2003a) and Xu et al. (2003b). In particular, negative correlation structures are also important for problems of biological, medical and physical nature; empirical examples of negative spatial autocorrelation can be found in Griffith (2019), Hu et al. (2018) and Ye et al. (2015). Most of the applications concerning spatial and spatio-temporal data analysis, characterised by negative correlation, are often described through hole effect models or damped oscillation models, as detailed by various authors (Ma and Jones, 2001; Journel and Froidevaux, 1982; Asghari, 2015). Moreover, besides the mining and geological applications, in the last years hole effect models have also been employed to describe the fluctuating spatial structure of functional magnetic resonance imaging data to enhance the detection of activated brain regions (Ye et al., 2015) or to model concentrations of airborne particulate matter (Alegría and Emery, 2024).

In the literature, several papers and textbooks have extensively discussed the classical properties of covariance functions (Chilés and Delfiner, 1999; Christakos, 1984; Longuet-Higgins, 1957; Journel and Huijbregts, 1981; Kamash and Robson, 1978; Matérn, 1980; Polya, 1949; Schoenberg, 1938; Stein, 1999; Yaglom, 1957), from which oscillatory covariance functions, resulting from the use of some Bessel functions or from the infinitely differentiable Bessel–Lommel functions, were proposed Yaglom (1987)

* Corresponding author.
E-mail addresses: sandra.deiaco@unisalento.it (De Iaco S.), donato.posa@unisalento.it (Posa D.).

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and Hristopulos (2015). Moreover, in addition to the well-known closure of the covariance class with respect to the sum, some linear combinations of continuous covariance functions, even with negative weights, were proved to be admissible covariance models (Vecchia, 1988; Gneiting, 2002; Hristopulos and Elogne, 2007; Ma, 2005; Gregori et al., 2008; Faouzi et al., 2020; Vargas-Guzmán et al., 2002; Posa, 2021; Alegría et al., 2024), leading to correlation models with negative values. In particular, the conditions to obtain a valid covariance from the difference of two real-valued covariance functions and, more generally, from the difference between complex-valued covariance functions can be found in Posa (2021, 2023a). Posa (2025) utilised the Whittle–Matérn family in order to define some classes of covariance models, suitable to model negative correlations, and their properties were analysed. Unlike other contributions, in these last papers a deep discussion on the behaviour of the proposed classes of models according to the parameter values was provided. Indeed, these classes of isotropic covariance models are very flexible in describing positive covariances as well as covariance functions which are negative in a subset of their domain (with only one zero), according to the respective parameter values and can be characterised by a linear or a parabolic behaviour near the origin. However these aspects were analysed only for some isotropic covariance models, defined on the usual Euclidean dimensional spaces ($\mathbb{R}$, $\mathbb{R}^2$ and $\mathbb{R}^3$). Thus, the extension to families of covariance functions on the d-dimensional domain, $\mathbb{R}^d$, and other specific analytic features, such as their absolute minimum values, need to be explored. Even in the work of Ma (2005), there are some qualitative comments on the behaviour of the proposed models, but there is no mention about the absolute minimum values that the models can reach.

In this paper, starting from three wide and commonly used families of isotropic covariance models (Gaussian, exponential and rational models), defined on $\mathbb{R}^d$, for any $d \in \mathbb{N}_+$, the conditions of the admissibility of their weighted differences have been derived. Thus, these classes represent a generalisation of the corresponding families of models in Posa (2021, 2023a) with respect to the dimension d of the Euclidean space $\mathbb{R}^d$. In addition, apart from the positive definiteness conditions of the proposed classes and some properties related to behaviour near the origin and sign, the novelty of the results (not found in the previous papers) is also referred to another analytical feature of the models, such as the functional form of the absolute minimum, which has been given for any Euclidean dimension d of the space. In particular, it is shown how the dimension of the Euclidean space impacts the minimum. Note that these analytical aspects of the models can be crucial in selecting the appropriate class for the empirical covariance function and then in the modelling stage. The more analytical information the analyst has, the more appropriate the choice of the model can be. Indeed, the studied families present a parametrisation that points out the relationship between the ratio of the scale parameters of the two covariance functions involved in the difference and the ratio of two non-negative multiplicative factors of the covariance functions involved in the same difference. A different parametrisation was considered for the Ma models, where the linear combination was obtained on the basis of one parameter that can assume negative values. It is also worth noting that since in Posa (2021, 2023a) the results were limited to some specific Euclidean dimensional spaces, the admissibility conditions were verified by recovering the spectral density in the dimensional space $\mathbb{R}^2$ or $\mathbb{R}^3$ from the spectral density in $\mathbb{R}$. On the other hand, in the present paper the results are valid in $\mathbb{R}^d$, not necessarily restricted to the special cases $d \leq 3$ and the spectral density is not derived from the one in $\mathbb{R}$.

The paper is organised as follows. In Section 2, a theoretical framework for the classes of continuous covariance functions constructed through the difference of two continuous families of covariance functions has been provided. Section 3 is devoted to introduce some general admissibility conditions for isotropic covariance models, defined on a spatial domain $\mathbb{R}^d$ for any $d \in \mathbb{N}_+$, which are obtained through the difference of three well-known standard models, such as the Gaussian, exponential and rational models. In Section 4, the absolute minimum values of the proposed families of covariance models have been given, as a function of the dimension $d \in \mathbb{N}_+$ of the Euclidean dimensional space $\mathbb{R}^d$. In Section 5, the performance of some models with negative values in $\mathbb{R}$, $\mathbb{R}^2$ and $\mathbb{R}^3$ has been assessed using simulated spatial data. For this purpose, the resulting statistics have denoted a significant improvement in the estimation performance obtained through the models that capture negative covariance values with respect to the model that decays monotonically. In Section 6, the estimation reliability of a linear combination of the proposed models with negative values has also been assessed using a real data set related to the population density of an Italian region. Finally, some conclusions have been given in Section 7.

2. A theoretical framework

The family of continuous covariance functions is completely described through the results of Bochner's theorem (Bochner, 1959).

Indeed, a continuous stationary complex-valued function C, defined on $\mathbb{R}^d$ is a covariance function if and only if it is the Fourier transform of a finite and non decreasing measure F, i.e.,

$$C(\boldsymbol{x}) = \int_{\mathbb{R}^d} \exp(i\boldsymbol{\omega}^T\boldsymbol{x}) dF(\boldsymbol{\omega}). \tag{1}$$

A special characterisation of (1) outcomes from the absolute continuity of the function F, i.e.,

$$C(\boldsymbol{x}) = \int_{\mathbb{R}^d} \exp(i\boldsymbol{\omega}^T\boldsymbol{x}) f(\boldsymbol{\omega}) d\boldsymbol{\omega}, \tag{2}$$

where the spectral density $f(\boldsymbol{\omega}) \geq 0, \boldsymbol{\omega} \in \mathbb{R}^d$ and $f \in L^1(\mathbb{R}^d)$.

If $C \in L^1(\mathbb{R}^d)$, then the spectral density function is continuous, moreover:

$$f(\omega) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \exp(-i\boldsymbol{\omega}^T\boldsymbol{x}) C(\boldsymbol{x}) d\boldsymbol{x}. \tag{3}$$

As clarified in Posa (2021), utilising Bochner's Theorem, larger classes of continuous covariance functions can be constructed through the difference of two continuous families of covariance functions as specified hereafter.

Theorem 2.1 (*Posa 2021*). *Let $C_k : \mathbb{R}^d \to \mathbb{C}, k = 1, 2$, be covariance functions, for which the Bochner characterisation as in (2) is assumed:*

$$C_k(\boldsymbol{x}; \boldsymbol{\gamma_k}) = \int_{\mathbb{R}^d} \exp(i\boldsymbol{\omega}^T \boldsymbol{x}) f_k(\boldsymbol{\omega}; \boldsymbol{\gamma_k}) d\boldsymbol{\omega}, \quad k = 1, 2,$$

with $f_k(\boldsymbol{\omega}; \cdot) \geq 0, \forall \boldsymbol{\omega} \in \mathbb{R}^d$ and $\int_{\mathbb{R}^d} f_k(\boldsymbol{\omega}; \cdot) d\boldsymbol{\omega} < \infty, \quad k = 1, 2.$

Then, given the following weighted difference function

$$C(\boldsymbol{x}; \mathbf{V}) = A_1 C_1(\boldsymbol{x}; \boldsymbol{\gamma}_1) - A_2 C_2(\boldsymbol{x}; \boldsymbol{\gamma}_2), \quad \boldsymbol{x} = (x_1, \dots, x_d) \in \mathbb{R}^d, \tag{4}$$

where $\boldsymbol{\gamma}_1$ and $\boldsymbol{\gamma}_2$ are vectors of parameters, A_1, A_2 are positive coefficients and $\mathbf{V} = (A_1, A_2, \boldsymbol{\gamma_1}, \boldsymbol{\gamma_2})$, expressed as

$$C(\boldsymbol{x}; \mathbf{V}) = \int_{\mathbb{R}^d} \exp(i\boldsymbol{\omega}^T \boldsymbol{x})(A_1 f_1(\boldsymbol{\omega}; \boldsymbol{\gamma_1}) - A_2 f_2(\boldsymbol{\omega}; \boldsymbol{\gamma_2})) d\boldsymbol{\omega}, \tag{5}$$

this last is a covariance function if and only if $\forall \boldsymbol{\omega} \in \mathbb{R}^d$,

$$A_1 f_1(\boldsymbol{\omega}; \boldsymbol{\gamma_1}) - A_2 f_2(\boldsymbol{\omega}; \boldsymbol{\gamma_2}) \geq 0. \tag{6}$$

Note that the integrability of $A_1 f_1(\boldsymbol{\omega}; \boldsymbol{\gamma_1}) - A_2 f_2(\boldsymbol{\omega}; \boldsymbol{\gamma_2})$ is automatically fulfilled since f_1 and f_2 are assumed integrable.

Consequently, the families of covariance functions can be enlarged by checking the condition in (6), on the basis of the spectral density functions f_1 and f_2.

In the isotropic case, if

$$\int_0^\infty x^{d-1} |C(x)| dx < \infty, \quad d \in \mathbb{N}, d \geq 2, \tag{7}$$

where $x = \|\boldsymbol{x}\|$, then the existence of a spectral density f is ensured. Consequently, the covariance and the spectral density functions can be expressed, respectively, as follows:

$$C(x) = \frac{2(\pi)^{d/2}}{\Gamma(d/2)} \int_0^\infty \Lambda_m(\omega x) \omega^{d-1} f(\omega) d\omega, \qquad x > 0, \tag{8}$$

and

$$f(\omega) = \frac{1}{2^{d-1}(\pi)^{d/2} \Gamma(d/2)} \int_0^\infty \Lambda_m(\omega x) x^{d-1} C(x) dx, \qquad \omega \in \mathbb{R}, \tag{9}$$

where

$$\Lambda_m(\omega) = 2^{(d-2)/2} \Gamma(d/2) \frac{J_{(d-2)/2}(\omega)}{\omega^{(d-2)/2}},$$

and J is a Bessel function of order $(d-2)/2$.

As illustrated by Yaglom (1987), expression (8) can be generalised for isotropic correlation models: that is, $\rho(x) = C(x)/C(0)$ is an isotropic correlation function on $\mathbb{R}^d$ if and only if it can be written as follows:

$$\rho(x) = \int_0^\infty \Lambda_m(\omega x) dF(\omega), \quad \int_0^\infty dF(\omega) = 1.$$

Hence, for all x,

$$\rho(x) \geq \inf_{\omega \geq 0} \Lambda_m(\omega);$$

in the peculiar cases $d = 2$ and $d = 3$, the following lower bounds for ρ are given:

$$d = 2, \quad \rho(x) \geq \inf_{\omega \geq 0} J_0(\omega) \approx -0.403;$$

$$d = 3, \quad \rho(x) \geq \inf_{\omega \geq 0} \frac{sin(\omega)}{\omega} \approx -0.218.$$

It is worth recalling that for the admissibility condition of a function C to be an isotropic covariance in the Euclidean $\mathbb{R}^d$ space, it is then required to compute the function f as in (9) and check the non-negativity condition of the same function f.

Thus, Theorem 2.1 can be formulated for the isotropic case, as stated in the following Corollary.

Corollary 2.1 (*Posa (2023a)*). *Let $C_k : \mathbb{R}^d \to \mathbb{R}, k = 1, 2$, be isotropic covariance functions, such that*

$$C_k(x; \boldsymbol{\gamma}_k) = \frac{2(\pi)^{d/2}}{\Gamma(d/2)} \int_0^\infty \Lambda_m(\omega x) \omega^{d-1} f_k(\omega; \boldsymbol{\gamma}_k) d\omega, \qquad x > 0, \qquad k = 1, 2,$$

where C_k satisfies the condition in (7). The function

$$C(x; \mathbf{V}) = \frac{2(\pi)^{d/2}}{\Gamma(d/2)} \int_0^\infty \Lambda_m(\omega x) \omega^{d-1} [A_1 f_1(\omega; \boldsymbol{\gamma}_1) - a_2 f_2(\omega; \boldsymbol{\gamma}_2)] d\omega, \qquad x > 0 \tag{10}$$

is a covariance function if and only if $\forall \omega \in \mathbb{R}$,

$$A_1 f_1(\omega; \boldsymbol{\gamma}_1) - A_2 f_2(\omega; \boldsymbol{\gamma}_2) \geq 0, \quad \int_0^\infty (A_1 f_1(\omega; \boldsymbol{\gamma}_1) - A_2 f_2(\omega; \boldsymbol{\gamma}_2)) d\omega < +\infty. \tag{11}$$

The families of covariance models obtained through Theorem 2.1 are more flexible than most of the traditional models (such as the so-called hole effect models in Journel and Huijbregts (1981) and Chilés and Delfiner (1999) or the models in Ma (2005)) because:

- according to the values of their parameters, the new 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;
- it is possible to select covariance models which present various behaviours near the origin;
- it is possible to obtain negative correlation models characterised by just one zero;
- these classes of models do not require that the two covariance functions, used in the difference, are of the same functional form;
- these new classes of covariance models present an extremely simple formalism and can be easily adapted to several case studies.

Unlike the family of models obtained through Theorem 2.1, most common classes of covariance models characterised by negative values always present the same features, such as a parabolic behaviour near the origin and countably infinitely many zeros; moreover, they are not able to describe different structures modifying the values of their parameters. Also the models with negative correlations, proposed by Gneiting (2002) starting from compactly supported correlation functions, have a parabolic behaviour near the origin.

Note that the families of correlation functions proposed by Posa (2023a) with the further generalisations introduced in this paper, are also able to model a linear behaviour near the origin; moreover, within the same class, it is possible to select correlation functions which are always positive in their domain, as well as correlation functions characterised by negative values in a subset of their domain, according to the parameters values on which the same models depend. Moreover, differently from Ma (2005), the formulation of these classes of models does not generally assume that the difference of two covariance functions is based on models with the same functional form.

In the multivariate context, Alegría and Emery (2024) provided new parametric families of isotropic matrix-valued functions exhibiting non-monotonic behaviours. Although an intersection can be found with respect to what was proposed in Posa (2023a), not all the classes of models (also in the complex domains) derived from Corollary 2.1 can be included in the results of Alegría and Emery (2024).

In addition, in Posa (2023a,b), some families of isotropic covariance models were obtained through the difference between Gaussian, exponential or rational isotropic covariance functions and the admissibility conditions, together with various analytic features of these covariance models were provided for the spatial domains $\mathbb{R}^d$, where $d \leq 3$. In these peculiar cases, the admissibility condition for the function C to be an isotropic covariance was computationally convenient, since it was enough to

- find the inverse Fourier transform f_1 of the function C in $\mathbb{R}$,
- calculate the corresponding multidimensional spectral density f (for $d = 2$ or $d = 3$) from f_1,
- and check if the function f is non negative.

In the following, a generalisation of these families of models with respect to the dimension d of the Euclidean space $\mathbb{R}^d$ is provided, as well as a discussion on some analytical features and on the functional forms of their absolute minimum, which is shown to be dependent on the dimension of the Euclidean space.

3. Isotropic covariance differences in any spatial dimension: admissibility and some features

This section is devoted to provide some general admissibility conditions for isotropic covariance models, defined on a spatial domain $\mathbb{R}^d$ for any $d \in \mathbb{N}_+$, which are obtained through the difference of three well-known standard models, such as the Gaussian, exponential and rational models.

Note that the following notation will be utilised hereafter: $\mathbf{V} = (A_1, A_2, \gamma_1, \gamma_2)$, with $A_1, A_2, \gamma_1, \gamma_2 > 0$, $\boldsymbol{x} = (x_1, x_2, \ldots, x_m) \in \mathbb{R}^d$, $x = \|\boldsymbol{x}\|$.

Theorem 3.1. *Given two isotropic Gaussian covariance functions, C_1 and C_2, defined on $\mathbb{R}^d$, which are characterised by the scale parameters γ_1 and γ_2, respectively, the following function C obtained through the weighted difference between C_1 and C_2*

$$C(x; \mathbf{V}) = A_1 e^{-\gamma_1 x^2} - A_2 e^{-\gamma_2 x^2}, \tag{12}$$

is a family of admissible isotropic covariance models in $\mathbb{R}^d$ for any $d \in \mathbb{N}_+$ if and only if the following relationship is satisfied:

$$1 \leq \gamma_1/\gamma_2 \leq (A_1/A_2)^{2/d}. \tag{13}$$

The proof can be found in Appendix A.1.

Note that (12) always presents just one zero for $x > 0$, therefore it always assumes negative values in a subset of $\mathbb{R}$ and presents a parabolic behaviour near the origin, because $C'(0) = 0$.

The admissibility condition is given for the weighted difference of two exponential covariance functions, as specified below.

Theorem 3.2. *Given two isotropic exponential covariance functions, C_1 and C_2, defined on $\mathbb{R}^d$, which are characterised by the scale parameters γ_1 and γ_2, respectively, the following function C obtained through the weighted difference between C_1 and C_2*

$$C(x;\mathbf{V}) = A_1 e^{-\gamma_1 x} - A_2 e^{-\gamma_2 x}, \tag{14}$$

is a family of admissible isotropic covariance models in $\mathbb{R}^d$ for any $d \in \mathbb{N}_+$ if and only if the following relationship is satisfied:

$$1 \leq \frac{\gamma_2}{\gamma_1} \leq \frac{A_1}{A_2}, \quad or \quad 1 \leq \frac{\gamma_1}{\gamma_2} \leq \left(\frac{A_1}{A_2}\right)^{1/d}. \tag{15}$$

Its proof is provided in Appendix A.2.

According to the parameters values, the family (14) can assume positive or negative values, as well as a linear or parabolic behaviour near the origin. In particular, it presents

- always positive values, linear behaviour and upwards concavity near the origin if $1 < \frac{\gamma_2}{\gamma_1} \leq \frac{A_1}{A_2}$, because $C'(0^+) < 0, C''(0^+) > 0$, or
- always positive values, parabolic behaviour and downwards concavity near the origin when $1 < \frac{\gamma_2}{\gamma_1} = \frac{A_1}{A_2}$, because $C'(0^+) = 0, C''(0^+) < 0$, or
- negative values in a subset of its domain, linear behaviour and upwards concavity near the origin if $1 < \frac{\gamma_1}{\gamma_2} < \left(\frac{A_1}{A_2}\right)^{1/d}$, because $C'(0^+) < 0, C''(0^+) > 0$.

Finally, it is also interesting to provide the admissibility condition for the case of the weighted difference of two rational covariance functions.

Theorem 3.3. *Let C_1 and C_2 be two isotropic rational covariance functions, defined on $\mathbb{R}^d$, which are characterised by the scale parameters γ_1 and γ_2, respectively. The following difference based on the two isotropic classes of rational covariance functions*

$$C(x;\mathbf{V}) = \frac{A_1}{(x^2+\gamma_1^2)^{(d+1)/2}} - \frac{A_2}{(x^2+\gamma_2^2)^{(d+1)/2}}, \tag{16}$$

is an admissible family of isotropic covariance functions if and only if

$$\gamma_2 \geq \gamma_1 \quad and \quad \frac{A_2}{A_1} \leq \frac{\gamma_2}{\gamma_1}. \tag{17}$$

The proof can be found in Appendix A.3.

According to the parameters values, the family (16) always presents a parabolic behaviour near the origin (because $C'(0) = 0$) and it assumes just positive values if $\frac{A_2}{A_1} \leq 1 < \frac{\gamma_2}{\gamma_1}$, otherwise it assumes negative values in a subset of its domain, if $1 < \frac{A_2}{A_1} < \frac{\gamma_2}{\gamma_1}$.

If $C(0) = 1$, the above mentioned families are referred to correlation models. In the following, the notation C is used independently to indicate the covariance or the correlation function.

4. Absolute minimum values of difference-based covariance models

In this section, the absolute minimum values of three wide families of covariance models based on the difference of Gaussian, exponential and rational models, have been determined, as a function of the dimension $d \in \mathbb{N}_+$ of the Euclidean space $\mathbb{R}^d$. These results are particularly useful, since it can be pointed out how fast the absolute minimum decays as the dimension d increases. Then, as a special case, the absolute minimum values for different dimensions of the domain ($\mathbb{R}$, $\mathbb{R}^2$, $\mathbb{R}^3$) have been provided. For these last cases, a comparison with respect to the already known minimum values of the models based on the Bessel functions, such as the smoothed cosine and the cardinal sine, can be presented and can help users in the selection of the most appropriate model to be fitted to the specific estimated correlation structure.

The proofs of the theoretical results given in the following sections have been given in Appendix B.

4.1. Difference between two Gaussian models

Given the family of isotropic correlation functions in (12), with $A_1 - A_2 = 1$ and $1 < \gamma_1/\gamma_2 < (A_1/A_2)^{2/d}$, then it can be easily verified that the minimum value, for a fixed value of the parameter vector $\mathbf{V}$, of the correlation function is:

$$C(x_m) = A_2\left[\frac{A_1}{A_2}\left(\frac{\gamma_1 A_1}{\gamma_2 A_2}\right)^{-\frac{\gamma_1}{\gamma_1-\gamma_2}} - \left(\frac{\gamma_1 A_1}{\gamma_2 A_2}\right)^{-\frac{\gamma_2}{\gamma_1-\gamma_2}}\right], \tag{18}$$

where $x_m = \sqrt{\frac{1}{\gamma_1-\gamma_2}\ln\left(\frac{\gamma_1 A_1}{\gamma_2 A_2}\right)}$.

Although x_m and $C(x_m)$ do not depend on the dimension of the Euclidean space $\mathbb{R}^d$, it is shown hereafter that the absolute minimum is a function of the domain dimension and it is less and less negative as the dimension increases. Note also that the minimum can be reached as $\gamma_1/\gamma_2 \to (A_1/A_2)^{2/d}$ and $(A_1/A_2)^{2/d} \to 1$.

Theorem 4.1. *Let C be the family of isotropic correlation functions in (12), defined on $\mathbb{R}^d$, with $A_1 - A_2 = 1$, $1 < \gamma_1/\gamma_2 < (A_1/A_2)^{2/d}$ and $d \in \mathbb{N}_+$; then the absolute minimum of C, with parameter vector $\mathbf{V}$, is given below:*

$$\min_{\mathbf{V}} C(x_m) = -\frac{2}{d\exp(\frac{d+2}{2})}. \tag{19}$$

It is worth highlighting that the absolute minimum given in (19) for the difference of isotropic Gaussian covariance functions, in $\mathbb{R}^d$ (for any d) can be specialised for the usual Euclidean domains ($\mathbb{R}, \mathbb{R}^2$ and $\mathbb{R}^3$), as specified hereafter:

- for $d = 1$, the absolute minimum value for $C(x_m)$ is equal to -0.4453;
- for $d = 2$, the absolute minimum value for $C(x_m)$ is equal to -0.1355 (the same minimum value reached by the covariance family defined as difference of two exponential models in $\mathbb{R}$);
- for $d = 3$, the absolute minimum value for $C(x_m)$ is equal to -0.0547.

4.2. Difference between two exponential models

Given the family of correlation functions in (14), with $A_1 - A_2 = 1$ and $1 < \gamma_1/\gamma_2 < (A_1/A_2)^{1/d}$, then the absolute minimum value $C(x_m)$ is the same as in (18), where $x_m = \frac{1}{\gamma_1-\gamma_2}\ln\left(\frac{\gamma_1 A_1}{\gamma_2 A_2}\right)$. Note that x_m and $C(x_m)$ do not depend on the dimension d of the Euclidean space $\mathbb{R}^d$; however, it is shown hereafter that the absolute minimum is a function of the domain dimension and it is less and less negative as the dimension d increases. Note also that the minimum can be reached as $\gamma_1/\gamma_2 \to (A_1/A_2)^{1/d}$ and $(A_1/A_2)^{1/d} \to 1$.

Theorem 4.2. *Let C be the family of isotropic correlation functions as in (14), defined on the domain $\mathbb{R}^d$, with $A_1 - A_2 = 1$, $1 < \gamma_1/\gamma_2 < (A_1/A_2)^{1/d}$ and $d \in \mathbb{N}_+$, then the absolute minimum of C, with parameter vector $\mathbf{V}$, is given below:*

$$\min_{\mathbf{V}}[C(x_m)] = -\frac{1}{d\exp(d+1)}. \tag{20}$$

Consequently, the minimum given in (20), is computed specifically for the Euclidean domains $\mathbb{R}, \mathbb{R}^2$ and $\mathbb{R}^3$, as detailed hereafter:

- for $d = 1$, the absolute minimum value for $C(x_m)$ is equal to -0.135 (the same absolute minimum value reached by the covariance family defined as difference of two Gaussian models in $\mathbb{R}^2$);
- for $d = 2$, the absolute minimum value for $C(x_m)$ is equal to -0.025;
- for $d = 3$, the absolute minimum value for $C(x_m)$ is equal to -0.006.

4.3. Difference between two rational models

Given the family of correlation functions in (16), with $\frac{A_1}{\gamma_1^{d+1}} - \frac{A_2}{\gamma_2^{d+1}} = 1$ and $1 < A_2/A_1 < \gamma_2/\gamma_1$, its absolute minimum value is obtained for $x_m = \sqrt{\frac{\gamma_2^2 - (\frac{A_2}{A_1})^{2/(d+3)}\gamma_1^2}{(\frac{A_2}{A_1})^{2/(d+3)} - 1}}$, as specified below:

$$\begin{aligned} C(x_m) &= \frac{A_1}{\left[\frac{\gamma_2^2 - (\frac{A_2}{A_1})^{2/(d+3)}\gamma_1^2}{(\frac{A_2}{A_1})^{2/(d+3)} - 1} + \gamma_1^2\right]^{\frac{d+1}{2}}} - \frac{A_2}{\left[\frac{\gamma_2^2 - (\frac{A_2}{A_1})^{2/(d+3)}\gamma_1^2}{(\frac{A_2}{A_1})^{\frac{2}{d+3}} - 1} + \gamma_2^2\right]^{\frac{(d+1)}{2}}} \\ &= \left[\left(\frac{A_2}{A_1}\right)^{\frac{2}{d+3}} - 1\right]^{\frac{d+1}{2}} \cdot \left[\frac{A_1(A_2/A_1)^{(d+1)/(d+3)} - A_2}{(A_2/A_1)^{(d+1)/(d+3)}}\right] \cdot \left[\frac{1}{(\gamma_2^2 - \gamma_1^2)^{(d+1)/2}}\right] \\ &= \left[\left(\frac{A_2}{A_1}\right)^{\frac{2}{d+3}} - 1\right]^{\frac{d+1}{2}} \cdot \left[\frac{A_1}{\gamma_1^{d+1}}\right] \cdot \left[\frac{(A_2/A_1)^{(d+1)/(d+3)} - (A_2/A_1)}{(A_2/A_1)^{(d+1)/(d+3)}}\right] \cdot \left[\frac{1}{(\frac{\gamma_2^2}{\gamma_1^2} - 1)^{(d+1)/2}}\right]. \end{aligned} \tag{21}$$

Differently from the other cases, both x_m and $C(x_m)$ depend on the dimension d of the Euclidean space $\mathbb{R}^d$. In the following, it is shown that even the absolute minimum is a function of the domain dimension and it is less and less negative as the dimension increases. Note also that the minimum can be searched for as $\gamma_2/\gamma_1 \to (A_2/A_1)$ and as $(A_1/A_2) \to 1$.

Theorem 4.3. *Let C be the family of correlation functions as in (16), defined on the domain $\mathbb{R}^d$, with $\frac{A_1}{\gamma_1^{d+1}} - \frac{A_2}{\gamma_1^{d+1}} = 1$, $1 < (A_2/A_1) < (\gamma_2/\gamma_1)$ and $d \in \mathbb{N}_+$, then the absolute minimum of C, with parameter vector $\mathbf{V}$, is given below:*

$$\min_{\mathbf{V}}[C(x_m)] = -\frac{2}{d(d+3)^{(d+3)/2}}. \tag{22}$$

It is worth highlighting that the minimum given in (22) for the difference of isotropic rational covariance functions, in $\mathbb{R}^d$ (for any d) can be specialised for one-two or three-dimensional domains ($\mathbb{R}, \mathbb{R}^2$ and $\mathbb{R}^3$), as clarified below:

- for $d = 1$, the absolute minimum value for $C(x_m)$ is equal to -0.125;
- for $d = 2$, the absolute minimum value for $C(x_m)$ is equal to -0.0179;
- for $d = 3$, the absolute minimum value for $C(x_m)$ is equal to -0.00309.

4.4. *Contribution with respect to existing literature*

In this section, some specific remarks regarding the contribution provided with respect to the existing results have been clarified.

- It is well known that the traditional hole effects covariance models (which stem from the $J_{(d-2)/2}$ Bessel functions) present characteristics completely different from the covariance families proposed in this paper: indeed the whole mentioned class of hole effects covariance models presents a countable infinity of zeros and a parabolic behaviour near the origin. On the other hand, the covariance families detailed in this paper have been constructed through the difference of covariance models and are characterised by just one zero, moreover they are able to describe different behaviours near the origin, not only parabolic, but also a linear behaviour.
- Gneiting (2002) proposed compactly supported correlation functions, which parametrise the smoothness of the associated stationary and isotropic random field as well as some ramifications to model negative correlations. Through the turning band operator, which preserves both compact support and the local behaviour of the correlation function at the origin, the following model
$$\rho(x) = \left[1 + \nu x - \frac{(\nu+1)(\nu+2+d)x^2}{d}\right](1-x)_+^{\nu}$$
was obtained which is an admissible correlation function in $\mathbb{R}^d$ if and only if $\nu \geq (d+5)/2$; note that the above model is characterised by just one zero and a parabolic behaviour near the origin. Moreover, in the same paper a further approach, in order to model compactly supported correlation functions with negative values, was given through the product of a compactly supported non-negative correlation function with a Bessel correlation function. Even in this last case, the whole family has a parabolic behaviour near the origin.
- The obtained results in the univariate case, in Sections 3 and 4, have their own worthiness and can support further developments aimed at enriching the class of covariance functions. The innovative results also consist of the definition of the functions that describe the absolute minimum of the introduced admissible functions. For instance, in the contribution of Ma (2005) there is a qualitative comment on the behaviour of the proposed model, but there is no mention about the absolute minimum values that the models can reach. Note also that these analytical aspects of the models can turn out to be crucial in selecting the appropriate class for the empirical covariance and then in the modelling stage. The more analytical information the analyst has, the more appropriate the choice of the model can be.
- The studied families, which can be derived from Corollary 2.1, present a parametrisation that points out the relationship between the ratio of the scale parameters (γ_1 and γ_2) of the two covariance functions involved in the difference and the ratio of two non-negative multiplicative factors (A_1 and A_2) of the covariance functions involved in the same difference. A different parametrisation was considered for the Ma models, where the linear combination was obtained on the basis of the parameter θ and $(1-\theta)$, assuming that θ could also be negative. Note also that in the Ma models, the linear combination is obtained by considering functions which belong to the same class, on the other hand, the families that can be derived from Corollary 2.1 do not require in general that the covariance functions C_1 and C_2 belong to the same class.
- In Posa (2023a), the results were limited to some specific Euclidean dimensional spaces and for the admissibility condition of the function C in the peculiar cases, it was enough to obtain the spectral density in a higher dimensional space $\mathbb{R}^2$ or $\mathbb{R}^3$ from the spectral density in $\mathbb{R}$. On the other hand, in the present paper the results are valid in $\mathbb{R}^d$, not necessarily restricted to the special cases $d \leq 3$ and the spectral density is not derived from the one in $\mathbb{R}$.
- The main aim of the paper written by Alegría and Emery (2024) consists of proposing new parametric families of isotropic matrix-valued functions exhibiting non-monotonic behaviours, namely hole effects and cross-dimples. Thus, although there is an intersection between what is proposed in Theorems 3.1 and 3.3 in the univariate case, and the Alegría et al. (2024), the proofs given require a different setting with respect to the proof of the positive definiteness condition in the multivariate case given in Alegría et al. (2024). Indeed, not all the classes of models proposed are included in the results of these authors.

5. A comparison of the models features

In this section, the characteristics presented in the previous sections for each covariance model are discussed.

First of all, it is reasonable to emphasise that the admissibility conditions of the classes of covariance models (12) and (14) depend on the dimension d of the domain and on their parameters $(\gamma_1, \gamma_2, A_1, A_2)$, denoted with the vector $\mathbf{V}$, as specified in Theorems 3.1 and 3.2. Regarding the other features, it is interesting to underline that, unlike the weighted difference of Gaussian covariance models (which can always be negative in a subset of the real domain and parabolic near the origin), the weighted difference of exponential covariance models can always be positive (with linear or parabolic behaviour near the origin) or negative in an interval of values (with linear behaviour near the origin). Note also that the conditions under which both models are negative are influenced by the dimension of the Euclidean space d, other than the values of vector $\mathbf{V}$ of parameters. Indeed, the ratio of the scale parameters γ_1/γ_2 must be between 1 and $(A_1/A_2)^{2/d}$ in the Gaussian case, and between 1 and $(A_1/A_2)^{1/d}$ in the exponential case; thus, the dimension d has effect in the definition of the upper bound.

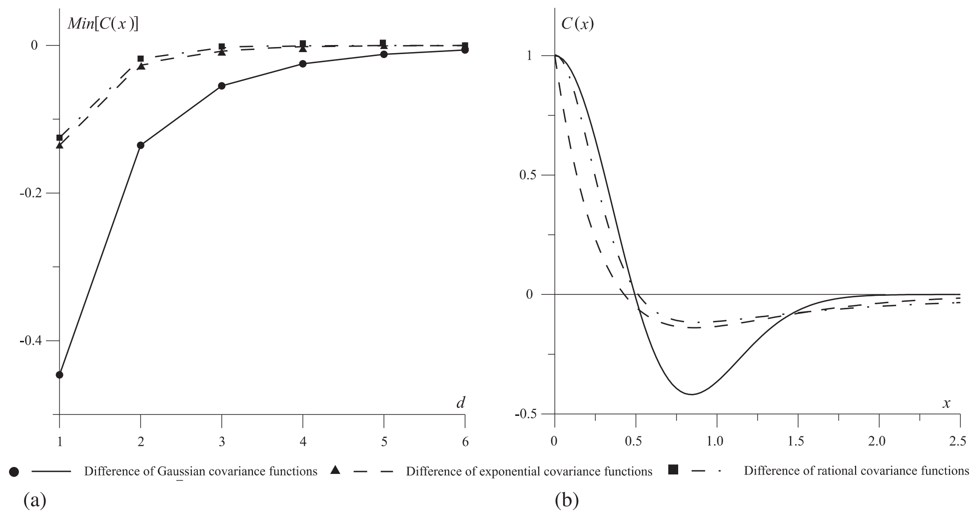

Fig. 1. (a) Minimum functions; (b) covariance functions in $\mathbb{R}$ ($d = 1$) for three families of models.

On the other hand, the inequality that defines the validity condition for the class of covariance functions in (16), obtained through the difference between rational models, only depends on the parameters $(\gamma_1, \gamma_2, A_1, A_2)$, as clarified in Theorem 3.3. In this case, the dimension of the Euclidean space $\mathbb{R}^d$ contributes in the definition of the class of models itself and does not influence the admissibility condition and the other characteristics of the family, such as the behaviour near the origin (which is always parabolic) and the sign of the models (which can always be positive or alternatively negative in a subset of the real domain).

Moreover, taking into account that the interest of these covariance functions stems from the possibility to assume negative values in a subset of their field of definition, which can be useful in many applications, it is important to underline that the extreme minimum values depend only on the dimension of the Euclidean space. In Fig. 1, the minimum values that each of the proposed models can assume are compared, as well as the covariance functions in $\mathbb{R}$ ($d = 1$) for the three families of models. The results discussed above represent some theoretical and practical advances particularly useful in the modelling stage, since they allow analysts to identify the most appropriate covariance model when the analysed data present correlation structure with positive or negative values.

6. A performance assessment

In this section, the performance of some models with negative values has been assessed using simulated spatial data and a real data set that refers to the population density of an Italian region.

6.1. Simulation results

The estimation ability of the class of models generated through the weighted difference of Gaussian models has been analysed in $\mathbb{R}$, $\mathbb{R}^2$ and $\mathbb{R}^3$ and a comparison with respect to the Gaussian model has been presented. To this aim, 300 data sets have been generated (through the Cholesky decomposition simulation algorithm) in the most common Euclidean dimensional spaces, $\mathbb{R}$, $\mathbb{R}^2$ and $\mathbb{R}^3$, that is, over the domains of the form $[0, n_1]/5$, with $n_1 = 500$ (that is, from 0 to 100, with step equal to 0.25), a grid $[0, n_2]/5 \times [0, n_2]/5$, with $n_2 = 19$ also denoted with $[0, n_2]^2/5$, (that is, 20×20, with horizontal/vertical step equal to 0.2), a grid $[0, n_3]^3/5$, with $n_3 = 9$ (that is, $10 \times 10 \times 10$, with step equal to 0.2), respectively. The simulated data, referred to the above-mentioned set of points regularly distributed on the domains, have been divided into the input data and the test data for the subsequent analysis. The corresponding geometry of the points allows the computation of the performance of the models for a wide range of distances between the test points and the input data points (falling in the neighbourhood), compatible with various sampling structures that can be encountered in practice. Moreover, given the geometry of the points, the estimation reliability can be evaluated for some test data whose closer neighbours are also at distances associated with the minimum value of the new proposed covariance models, which can be of interest for real applications.

The models constructed through the weighted difference of Gaussian models in $\mathbb{R}$, $\mathbb{R}^2$ and $\mathbb{R}^3$ and used for simulation (Fig. 2-a), are given below:

$$C_1(x) = 6.9\, exp(-7x^2) - 5.9\, exp(-6x^2), \quad (23)$$

$$C_2(x) = 20.1\, exp(-7.44x^2) - 19.1\, exp(-7.19x^2), \quad (24)$$

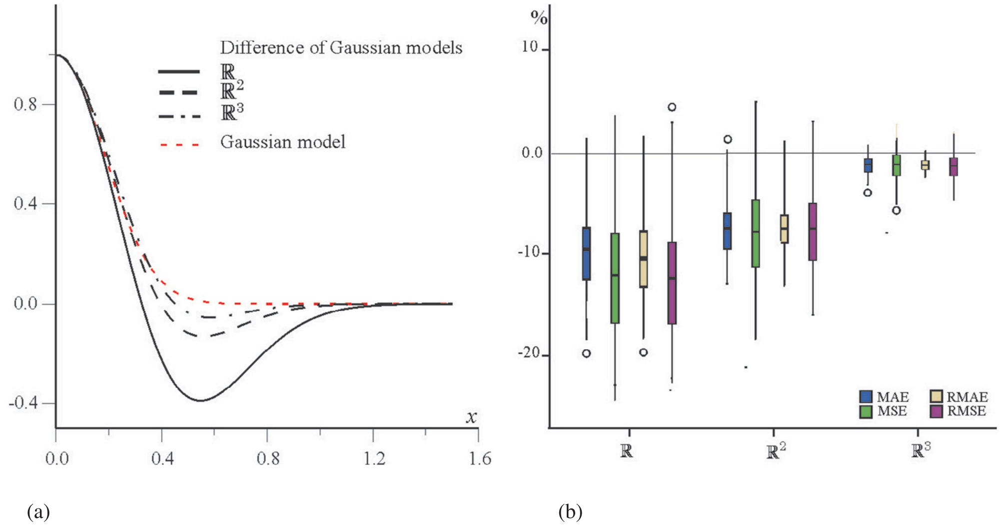

Fig. 2. (a) isotropic covariance models in $\mathbb{R}$, $\mathbb{R}^2$, $\mathbb{R}^3$; (b) box-plot of the relative improvement (in %) of the error indexes computed for the difference of Gaussian models and the traditional Gaussian model.

$$C_3(x) = 30.1\, exp(-5.33x^2) - 29.1\, exp(-5.01x^2). \tag{25}$$

The reliability of the models has been evaluated through the jackknife results. In detail, each simulated data set has been splitted in two subsets: the input data for kriging and the test data, also called jackknife data. These last include the points where the estimates have to be computed (through kriging) and the simulated data to be used for comparison. The improvement in terms of estimation reliability, with respect to the Gaussian model, has been evaluated even for the points whose closer neighbours are also at distances associated with the minimum value of the new proposed covariance models. Thus, the discrepancies between the estimation performance obtained through the jackknife, determined by using the models in (23), (24) and (25) and the one derived by using the Gaussian model $C(x) = exp(-3x^2/0.2)$ (Fig. 2-a), have been computed.

The assessment of the estimation performances concerning the models with negative values has been carried out through four different indicators of the errors, namely the mean absolute error (MAE), the root mean square error (MSE), the relative mean absolute error (RMAE) and the relative root mean square error (RMSE), which have been calculated between the previously simulated values and the jackknife estimated ones (Table 1). Moreover, for each error indicator, a percentage relative variation (Δ) between the error indicators related to the estimates based on the difference models and the ones related to the estimates based on the Gaussian model have been computed in order to highlight the deviation, in terms of predictive performances. Indeed, negative values of Δ denote an improvement in performance obtained through models that capture negative covariance values with respect to a model that decays monotonically. A discussion on the advantages of using a covariance model with negative values, has been also based on the statistical T-test of the null hypothesis that there is, on average, no difference in terms of the error indexes ($\delta = 0$) and on the corresponding p-values.

The values of the error indicators concerning the estimations computed, respectively, for the domains $\mathbb{R}$, $\mathbb{R}^2$ and $\mathbb{R}^3$ with the models (23), (24) and (25) and the statistics, referred to the variation with respect to the use of a Gaussian model, are given in Table 1. From the reported results, it is evident that the kriging estimates obtained by using the models (23), (24) and (25) are more accurate than the one computed by adopting a monotonically decreasing model. This improvement is measured in terms of the percentage relative variation Δ, which remains negative for all the cases (in the range −13.574, −9.522% in a one-dimensional domain, −7.927, −6.633% in a two-dimensional domain and −2.520, −1.981% in a three-dimensional domain). It is worth highlighting that the deviations of predictive performances are even more negative if the index Δ is computed for the points whose closer neighbours are also at distances associated with the minimum value of the new proposed covariance models. In this last case, the Δ index decreases of approximately of 1.2–1.7 points.

Moreover, the test statistics and the p-value provide a further quantitative assessment of the improvement identified in the estimation process when the covariance models with the negative values are considered, which reflects in lower errors. The p-values (from 3.54E−13 to 0.0986) lead mainly to the rejection of the null hypothesis at the significance level of 10% for the three Euclidean spaces. Even for the estimations in the three dimensional domain, the p-values remain lower than the significance level for all the error indexes, with exception of the one related to the MAE. However, note that both the percentage relative variations Δ and the p-value levels take on values higher, as the spatial dimension increases, so that the performance improvement decreases and the rejection of the test becomes less and less statistically significant. This is due to the admissible absolute minimum of the covariance models with negative values, which tends to be closer to zero, when the Euclidean dimension increases (especially for spatial dimension d greater than three), making less relevant the discrepancy between the covariance models with negative values and the monotonically decaying models.

Table 1
Errors related to the estimates obtained through the difference models and the corresponding statistics referred to the variation with respect to a decaying Gaussian model.

	$\mathbb{R}$	$\mathbb{R}^2$	$\mathbb{R}^3$	$\mathbb{R}$	$\mathbb{R}^2$	$\mathbb{R}^3$
	Estimate errors			Δ (%)		
MAE	0.023	0.011	0.028	−9.522	−6.633	−1.981
MSE	0.031	0.037	0.038	−12.635	−7.927	−2.322
RMAE	0.113	0.099	0.119	−10.761	−6.786	−2.210
RMSE	0.127	0.105	0.128	−13.574	−7.563	−2.520
	Stat. test (Hp. $\delta = 0$)			p-value		
MAE	−6.565	−4.565	−1.529	4.47E−10	8.76E−06	0.1277
MSE	−7.620	−5.035	−1.687	1.03E−12	1.07E−06	0.0932
RMAE	−7.305	−4.885	−1.663	6.65E−12	2.13E−06	0.0978
RMSE	−7.797	−4.942	−1.742	3.54E−13	1.64E−06	0.0831

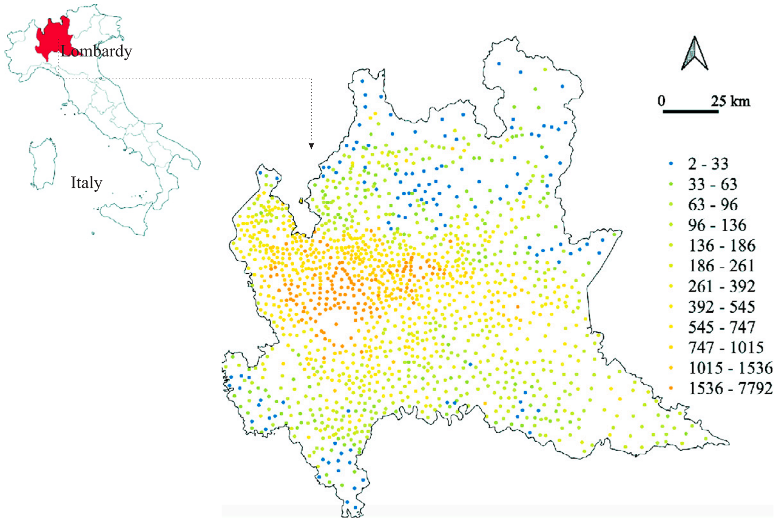

Fig. 3. Colour map of the population density values (per km^2), recorded in 2019 at 1505 municipalities of Lombardy Region (Northern Italy). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

6.2. An application to population density

In the present section, the spatial observations of a demographic variable, provided by the Italian Institute of Statistics (ISTAT), have been analysed. In Fig. 3, the population density values (per km^2) recorded in 2019 at 1505 municipalities of Lombardy region (Northern Italy) are illustrated. The data locations are distributed all over the region. The observations in between the first and second quartiles (96.36 and 746.91, respectively) are scattered throughout the domain. Apart from Milan, where the maximum density has been observed, other high density values have been registered in various other urban centres of the region, not only around the chiefdom, but also in some provincial capitals spread over the territory. On the other hand, the minimum densities have been found in the Northern part and in some sparse towns of the Southern area. The assessment of the adequacy of the fitted model has been evaluated through the leave-one-out cross-validation procedure as well as the jackknife technique where a subset of the available data has been used as validation set. The last has been obtained by randomly selecting 600 points (approximately 40%) from the complete data set.

The data are characterised by negative correlation; indeed, the estimated spatial covariance shows a linear behaviour near the origin, decreasing values and then negative values from the fourth spatial lag until the last one, corresponding approximately to 160 km (Fig. 4-a). On the basis of these characteristics, the sample covariance function has been modelled by a linear combination of two classes of isotropic covariances obtained on the one hand through the difference of exponential covariance functions in order to catch the linear behaviour near the origin and on the other hand through the difference of Gaussian covariance functions which is able to reproduce the depression in the covariance function, up to a minimum equal to −13.090. Thus, the corresponding parameters have been evaluated through graphical inspection and then the goodness of fit has been measured through some standard deviation indexes. In Fig. 4-(a), the sample covariance function computed for 10 spatial lags and the following fitted model

$$C(x) = 4800[8.2\exp(-3x/60) - 7.2\exp(-3x/64)] + 108000[1.23\exp(-(3x/90)^2) - 0.23\exp(-(3x/206)^2)] \quad (26)$$

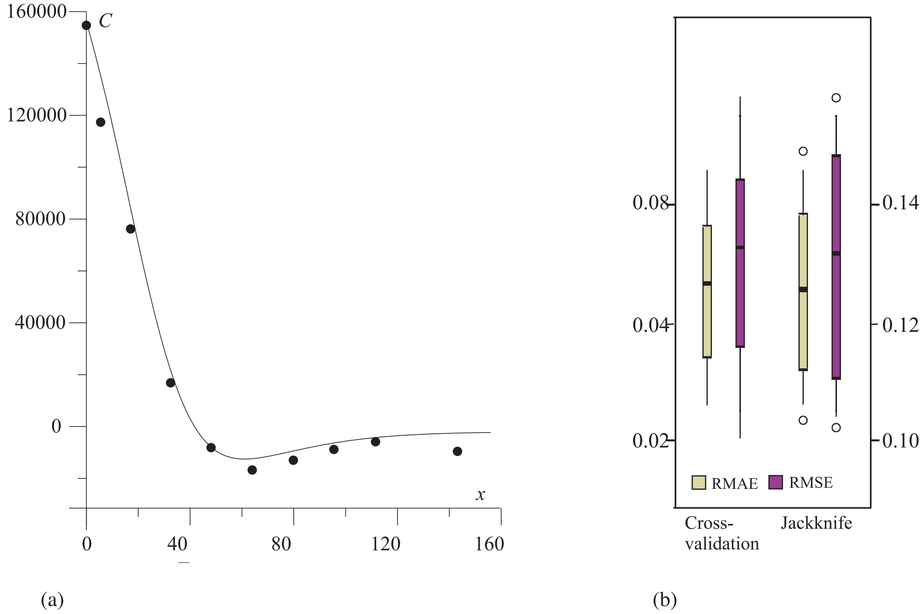

Fig. 4. (a) Sample covariance function and the fitted model for the population density of Lombardy (Italy); (b) box-plot of the error metrics for cross-validation and jackknife estimations.

are illustrated.

It is worth highlighting that the linear behaviour near the origin and the downward tendency with negative values until the last spatial lag exclude the traditional hole effect models, obtained through the Bessel function, since they present a parabolic behaviour near the origin and an infinite number of zeros. Note also that the parameters values, evaluated through visual inspection, $A_1 = 8.2$, $A_2 = 7.2$, $\gamma_1 = 3/60$, $\gamma_2 = 3/64$, for the difference of exponentials and $A_1 = 1.23$, $A_2 = 0.23$, $\gamma_1 = 3/90$, $\gamma_2 = 3/206$ for the difference of Gaussian satisfy the admissibility condition given in Theorems 3.1 and 3.2. Moreover, the relative error indexes RMAE and RMSE, computed for the cross-validation estimates and for the jackknife ones, are 0.06 and 0.13 (Fig. 4-b), thus they confirm its good performance in terms of estimation accuracy.

This application represents a classical example of spatial phenomenon characterised by negative correlation, since as the spatial lag increases, the relationships among the data values become discordant so that the corresponding correlation measure is negative. For this specific case study, this can be explained by the fact that the couples of points, fallen in these lags, involve big cities and the surrounding cities which are much smaller. It has also been verified that this behaviour is common to the data of the same variable collected for other areas, underlying that this can be considered a recurrent feature.

7. Conclusions

The absolute minimum of three wide families of covariance models based on difference between Gaussian, exponential and rational models, were determined as a function of the Euclidean domain dimension. On the basis of these results, it can be pointed out how fast the absolute minimum decays as the domain dimension increases. Then, as a special case, the absolute minimum values for different dimensions of the Euclidean space $\mathbb{R}$, $\mathbb{R}^2$ and $\mathbb{R}^3$ were provided. For these cases, a comparison with respect to the already known minimum values of the model based on the Bessel functions, such as the smoothed cosine (valid in $\mathbb{R}$) and the cardinal sine (valid, under some condition, up to $\mathbb{R}^3$), was presented, since it can help users in the selection of the most appropriate model to be fitted to the specific empirical correlation function.

Exploring all the theoretical features of these recent classes of models, characterised by negative correlation, allows the users to appreciate their effective flexibility during the fitting process. The performance of some models with negative values in $\mathbb{R}$, $\mathbb{R}^2$, and $\mathbb{R}^3$, was assessed using simulated spatial data. The statistics denoted a notable improvement of the estimation performance obtained through the models which capture the negative covariance values with respect to the model that decays monotonically. Moreover, the application of a linear combination of the difference of exponentials and the difference of Gaussian models to describe the spatial correlation with negative values to the population density of an Italian region highlights the real need of the proposed model.

These results can encourage the application of the proposed models from a practical point of view, for example in neuroscience or in demography, where some variables exhibit covariance functions, which generally show linear or parabolic behaviour near the origin and decreasing values that become negative at a spatial lag and remain negative until the last selected lag; this aspect represents the objective of future studies. As advances, the formulation of the covariance functions with negative values given in Posa (2023a) and the generalisation to the Euclidean space $\mathbb{R}^d$, proposed in the present paper together with a discussion on some analytical features, can represent the basis to further expand this class of models.

CRediT authorship contribution statement

De Iaco S.: Conceptualization, Data curation, Formal analysis, Funding acquisition, Methodology, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **Posa D.:** Conceptualization, Data curation, Formal analysis, Funding acquisition, Methodology, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Proofs on the admissibility conditions

A.1. Proof of Theorem 3.1

Let C_1 and C_2 be two isotropic Gaussian covariance functions, defined on $\mathbb{R}^d$, which are characterised by the scale parameters γ_1 and γ_2. Since $C_1 \in L^1(\mathbb{R}^d)$ and $C_2 \in L^1(\mathbb{R}^d)$, then their spectral density functions f_1 and f_2 exist and are continuous. Moreover, in the isotropic case, since the condition in (7) is satisfied, the spectral density of a Gaussian covariance function with scale parameter a is determined hereafter:

$$f(\omega) = K(\omega)\int_0^{\infty} J_{(d-2)/2}(\omega x)x^{d/2}e^{-ax^2}\,dx = \left(\frac{1}{4\pi a}\right)^{d/2} e^{-\omega^2/4a}, \tag{27}$$

where $\omega = \|\boldsymbol{\omega}\|$, $K(\omega)^{-1} = (2\pi)^{d/2}\omega^{(d-2)/2}$ and J is the Bessel function of order $(d-2)/2$ (Gradshteyn and Ryzhik, 2007). Thus, from the representation of the isotropic functions C_1 and C_2, it results that

$$A_1 f_1(\omega;\gamma_1) - A_2 f_2(\omega;\gamma_2) = \left(\frac{1}{4\pi}\right)^{d/2}\left[\frac{A_1}{\gamma_1^{d/2}}e^{-\omega^2/4\gamma_1} - \frac{A_2}{\gamma_2^{d/2}}e^{-\omega^2/4\gamma_2}\right]. \tag{28}$$

Since the function in (28) is integrable, it is non negative if and only if:

$$\frac{\omega^2}{4}\left(\frac{1}{\gamma_2} - \frac{1}{\gamma_1}\right) \geq \ln\left[\frac{A_2}{A_1}\left(\frac{\gamma_1}{\gamma_2}\right)^{d/2}\right]. \tag{29}$$

The condition in (29) is satisfied if and only if $\gamma_1 \geq \gamma_2$ and

$$\frac{A_2}{A_1}\left(\frac{\gamma_1}{\gamma_2}\right)^{d/2} \leq 1 \Leftrightarrow \frac{\gamma_1}{\gamma_2} \leq \left(\frac{A_1}{A_2}\right)^{2/d},$$

which proves the inequalities in (13). □

A.2. Proof of Theorem 3.2

Given two isotropic exponential covariance functions, C_1 and C_2 on $\mathbb{R}^d$, which are characterised by the scale parameters γ_1 and γ_2, then their spectral density functions f_1 and f_2 exist and are continuous, since $C_1 \in L^1(\mathbb{R}^d)$ and $C_2 \in L^1(\mathbb{R}^d)$. Moreover, taken into account that the condition in (7) is satisfied, the spectral density of an isotropic exponential covariance function with scale parameter a, is computed as follows:

$$f(\omega) = K(\omega) \int_0^\infty J_{(d-2)/2}(\omega x) x^{d/2} e^{-ax} dx = \frac{\Gamma(\frac{d+1}{2})}{\pi^{(d+1)/2}} \frac{a}{(a^2+\omega^2)^{(d+1)/2}}, \tag{30}$$

where $\omega = \|\boldsymbol{\omega}\|$, $K(\omega)^{-1} = (2\pi)^{d/2}\omega^{(d-2)/2}$, Γ is the Gamma function and J is the Bessel function of order $(d-2)/2$ (Gradshteyn and Ryzhik, 2007). On the basis of the spectral representation of the isotropic functions C_1 and C_2, then

$$\begin{aligned} &A_1 f_1(\omega;\gamma_1) - A_2 f_2(\omega;\gamma_2) \\ &= \frac{\Gamma(\frac{d+1}{2})}{\pi^{(d+1)/2}} \left[\frac{A_1\gamma_1}{(\gamma_1^2+\omega^2)^{(d+1)/2}} - \frac{A_2\gamma_2}{(\gamma_2^2+\omega^2)^{(d+1)/2}} \right]. \end{aligned} \tag{31}$$

Since the function in (31) is integrable, it is non negative if and only if:

$$\left(\frac{\gamma_2^2+\omega^2}{\gamma_1^2+\omega^2} \right)^{(d+1)/2} - \frac{A_2}{A_1}\frac{\gamma_2}{\gamma_1} \geq 0 \qquad \forall \omega \in \mathbb{R}. \tag{32}$$

Thus, if $\gamma_1 > \gamma_2$, the inequality in (32) is satisfied if and only if

$$1 < \frac{\gamma_1}{\gamma_2} \leq \left(\frac{A_1}{A_2} \right)^{1/d}.$$

On the other hand, if $\gamma_1 < \gamma_2$, the inequality in (32) is satisfied if and only if

$$1 < \frac{\gamma_2}{\gamma_1} \leq \frac{A_1}{A_2}.$$

If $\gamma_1 = \gamma_2$, then $A_1/\,A_2 \geq 1$ and $(A_1/\,A_2)^{1/d} \geq 1$. Then the condition in (15) is proved. □

A.3. Proof of Theorem 3.3

Consider that the spectral density of a rational covariance function with scale parameter a can be expressed as (Gradshteyn and Ryzhik, 2007):

$$f(\omega) = K(\omega) \int_0^\infty J_{(d-2)/2}(\omega x) x^{d/2} (x^2+a^2)^{-(d+1)/2} dx = W \frac{\exp(-a\omega)}{a}, \tag{33}$$

where $\omega = \|\boldsymbol{\omega}\|$, J is the Bessel function of order $(d-2)/2$,

$$K(\omega) = \frac{1}{(2\pi)^{d/2}\omega^{(d-2)/2}},$$

$W^{-1} = 2^d \pi^{(d-1)/2} \Gamma[(d+1)/2]$ and Γ the Gamma function (Gradshteyn and Ryzhik, 2007). Thus, from the representation of the isotropic covariance functions C_1 and C_2, it results that

$$A_1 f_1(\omega;\gamma_1) - A_2 f_2(\omega;\gamma_2) = W \left[\frac{A_1}{\gamma_1}\exp(-\gamma_1\omega) - \frac{A_2}{\gamma_2}\exp(-\gamma_2\omega) \right]. \tag{34}$$

Since the function in (34) is integrable, it is non negative if and only if:

$$\exp\left[\omega(\gamma_2-\gamma_1)\right] \geq \frac{A_2}{A_1}\frac{\gamma_1}{\gamma_2}, \qquad \forall \omega \in \mathbb{R}. \tag{35}$$

Thus, the inequality (35) is always satisfied if and only if $\gamma_1 \leq \gamma_2$ and $\frac{A_2}{A_1}\frac{\gamma_1}{\gamma_2} \leq 1$, hence the condition (17) is proved. □

Appendix B. Proofs on the absolute minimum functions

B.1. Proof of Theorem 4.1

Let $\Delta = \left(\frac{A_1}{A_2}\right)^{2/d}$, $\delta = \frac{\gamma_1}{\gamma_2}$ and $A_1 - A_2 = 1$, then $A_2 = \frac{1}{\Delta^{d/2}-1}$. It results

$$C(x_m) = \frac{1}{\Delta^{d/2}-1} \left[\Delta^{d/2} \left(\delta \Delta^{d/2} \right)^{-\frac{\delta}{\delta-1}} - \left(\delta\, \Delta^{d/2} \right)^{-\frac{1}{\delta-1}} \right].$$

The minimum can be found first of all as $\gamma_1/\gamma_2 \to (A_1/A_2)^{2/d}$, or equivalently as $\delta \to \Delta$, through the computation of the following limit:

$$\begin{aligned}
\lim_{\delta\to\Delta} C(x_m) &= \lim_{\delta\to\Delta} \frac{1}{\Delta^{d/2}-1}\left[\Delta^{d/2}\left(\delta\Delta^{d/2}\right)^{-\frac{\delta}{\delta-1}} - \left(\frac{\gamma_1}{\gamma_2}\Delta^{d/2}\right)^{-\frac{1}{\delta-1}}\right] \\
&= \frac{1}{\Delta^{d/2}-1}\left[\Delta^{d/2}\left(\Delta\cdot\Delta^{d/2}\right)^{-\frac{\Delta}{\Delta-1}} - \left(\Delta\cdot\Delta^{d/2}\right)^{-\frac{1}{\Delta-1}}\right] \\
&= \frac{\left(\Delta\cdot\Delta^{d/2}\right)^{-\frac{1}{\Delta-1}}}{\Delta^{d/2}-1}\left[\Delta^{d/2}\left(\Delta\cdot\Delta^{d/2}\right)^{-\frac{\Delta}{\Delta-1}+\frac{1}{\Delta-1}} - 1\right] \\
&= \frac{\left(\Delta\cdot\Delta^{d/2}\right)^{-\frac{1}{\Delta-1}}}{\Delta^{d/2}-1}\left[\frac{\Delta^{d/2}}{\Delta\cdot\Delta^{d/2}} - 1\right] = \frac{-\left(\Delta\cdot\Delta^{d/2}\right)^{-\frac{1}{\Delta-1}}(\Delta-1)}{(\Delta^{d/2}-1)\Delta} \\
&= \frac{-(\Delta-1)\Delta^{-\frac{(d+2)}{2(\Delta-1)}-1}}{\Delta^{d/2}-1} = \frac{-(\Delta-1)\Delta^{-\frac{(d+2R)}{2(\Delta-1)}}}{\Delta^{d/2}-1} \\
&= \frac{-(\Delta-1)\exp(-\frac{(d+2R)}{2(\Delta-1)}\ln\Delta)}{\Delta^{d/2}-1}.
\end{aligned}$$

Assuming $t = \Delta - 1$, the minimum value is reached by computing the limit of the above expression as $t \to 0^+$:

$$\begin{aligned}
&\lim_{t\to0^+} \frac{-t\exp[-\frac{(d+2t+2)}{2t}\ln(t+1)]}{(t+1)^{d/2}-1} \\
&= \left[\lim_{t\to0^+}\frac{-t}{(t+1)^{d/2}-1}\right]\cdot\left[\exp\left(\lim_{t\to0^+} -\frac{(d+2t+2)}{2}\right)\right]\cdot\left[\lim_{t\to0^+}\frac{\ln(t+1)}{t}\right] \\
&= \lim_{t\to0^+}\frac{-1}{d/2(t+1)^{\frac{d}{2}-1}}\exp\left(-\frac{d+2}{2}\right) = -\frac{2}{d\exp(\frac{d+2}{2})}. \quad \square
\end{aligned}$$

B.2. Proof of Theorem 4.2

Let $\Delta = \left(\frac{A_1}{A_2}\right)^{1/d}$, $\delta = \frac{\gamma_1}{\gamma_2}$ and $A_1 - A_2 = 1$, then it results that

$$C(x_m) = \frac{1}{\Delta^d - 1}\left[\Delta^d\left(\delta\Delta^d\right)^{-\frac{\delta}{\delta-1}} - \left(\delta\Delta^d\right)^{-\frac{1}{\delta-1}}\right].$$

The absolute minimum can be found first of all as $\gamma_1/\gamma_2 \to (A_1/A_2)^{1/d}$, or equivalently as $\delta \to \Delta$, which requires to compute the following limit

$$\begin{aligned}
\lim_{\delta\to\Delta} C(x_m) &= \lim_{\delta\to\Delta}\frac{1}{\Delta^d-1}\left[\Delta^d\left(\delta\Delta^d\right)^{-\frac{\delta}{\delta-1}} - \left(\delta\Delta^d\right)^{-\frac{1}{\delta-1}}\right] \\
&= \frac{1}{\Delta^d-1}\left[\Delta^d\left(\Delta\cdot\Delta^d\right)^{-\frac{\Delta}{\Delta-1}} - \left(\Delta\cdot\Delta^d\right)^{-\frac{1}{\Delta-1}}\right] \\
&= \frac{\left(\Delta\cdot\Delta^d\right)^{-\frac{1}{\Delta-1}}}{\Delta^d-1}\left[\frac{\Delta^d}{\Delta\cdot\Delta^d} - 1\right] = \frac{-\left(\Delta\cdot\Delta^d\right)^{-\frac{1}{\Delta-1}}(\Delta-1)}{(\Delta^d-1)\Delta} \\
&= \frac{-(\Delta-1)\Delta^{-\frac{(d+1)}{(\Delta-1)}-1}}{\Delta^d-1} = \frac{-(\Delta-1)\exp(-\frac{(d+\Delta)}{(\Delta-1)}\ln\Delta)}{\Delta^d-1}.
\end{aligned}$$

Assuming $t = \Delta - 1$, the minimum value is reached by computing the limit of the above expression as $t \to 0^+$:

$$\begin{aligned}
&\lim_{t\to0^+}\frac{-t\exp[-\frac{(d+t+1)}{t}\ln(t+1)]}{(t+1)^d-1} \\
&= \left[\lim_{t\to0^+}\frac{-t}{(t+1)^d-1}\right]\cdot\left[\exp\left(\lim_{t\to0^+} -(d+t+1)\right)\right]\cdot\left[\lim_{t\to0^+}\frac{\ln(t+1)}{t}\right] \\
&= \lim_{t\to0^+}\frac{-1}{d(t+1)^{d-1}}\exp[-(d+1)] = -\frac{1}{d\exp(d+1)}. \quad \square
\end{aligned}$$

B.3. Proof of Theorem 4.3

Let $\Delta = \left(\frac{A_2}{A_1}\right)$, $\delta = \left(\frac{\gamma_2}{\gamma_1}\right)$ and $\frac{A_1}{\gamma_1^{d+1}} - \frac{A_2}{\gamma_2^{d+1}} = 1$, then

$$\frac{A_1}{\gamma_1^{d+1}} = \frac{\delta^{d+1}}{\delta^{d+1} - \Delta}.$$

Consequently:

$$\begin{aligned}
C(x_m) &= \left[\Delta^{\frac{2}{d+3}} - 1\right]^{\frac{d+1}{2}} \cdot \left[\frac{\delta^{d+1}}{\delta^{d+1} - \Delta}\right] \cdot \left[\frac{\Delta^{(d+1)/(d+3)} - \Delta}{\Delta^{(d+1)/(d+3)}}\right] \cdot \left[\frac{1}{(\delta^2 - 1)^{(d+1)/2}}\right] \\
&= \left[\Delta^{\frac{2}{d+3}} - 1\right]^{\frac{d+1}{2}} \cdot \left[\frac{\delta^{d+1}}{\delta^{d+1} - \Delta}\right] \cdot \left[\frac{-\Delta^{(d+1)/(d+3)}(\Delta^{2/(d+3)} - 1)}{\Delta^{(d+1)/(d+3)}}\right] \cdot \left[\frac{1}{(\delta^2 - 1)^{(d+1)/2}}\right] \\
&= -\left[\Delta^{2/(d+3)} - 1\right]^{\frac{d+3}{2}} \cdot \left[\frac{\delta^{d+1}}{\delta^{d+1} - \Delta}\right] \cdot \left[\frac{1}{(\delta^2 - 1)^{(d+1)/2}}\right].
\end{aligned}$$

The absolute minimum can be found first of all as $(A_2/A_1) \to \gamma_2/\gamma_1$, or equivalently as $\Delta \to \delta$. Thus, the following limit is computed:

$$\begin{aligned}
\lim_{\Delta\to\delta} C(x_m) &= \lim_{\Delta\to\delta} -\left[\Delta^{2/(d+3)} - 1\right]^{\frac{d+3}{2}} \cdot \left[\frac{\delta^{d+1}}{\delta^{d+1} - \Delta}\right] \cdot \left[\frac{1}{(\delta^2 - 1)^{(d+1)/2}}\right] \\
&= -\left[\delta^{2/(d+3)} - 1\right]^{\frac{d+3}{2}} \left[\frac{\delta^{d+1}}{\delta^{d+1} - \delta}\right] \left[\frac{1}{(\delta^2 - 1)^{(d+1)/2}}\right] \\
&= -\left[\frac{\delta^d}{(\delta+1)^{(d+1)/2}(\delta^{d-1} + \delta^{d-2} + \cdots + \delta + 1)}\right] \left[\frac{\delta^{2/(d+3)} - 1}{\delta - 1}\right]^{(d+3)/2}.
\end{aligned}$$

On the basis of the above expression, the absolute minimum is reached as $\delta \to 1$ through the following limit:

$$\begin{aligned}
&- \lim_{\delta\to 1}\left[\frac{\delta^d}{(\delta+1)^{(d+1)/2}(\delta^{d-1} + \delta^{d-2} + \cdots + \delta + 1)}\right] \left[\frac{\delta^{2/(d+3)} - 1}{\delta - 1}\right]^{(d+3)/2} \\
&= -\left[\frac{1}{2^{(d+1)/2} d}\right] \cdot \left[\lim_{\delta\to 1} \frac{2}{(d+3)} \frac{\delta^{-(d+1)/(d+3)}}{1}\right]^{(d+3)/2} \\
&= -\frac{2}{d(d+3)^{(d+3)/2}}. \quad \square
\end{aligned}$$

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