Computing non-separability for space-time covariance functions: a case study on PM_{10} data

Calcolo della non separabilita' per funzioni di covarianza spazio-temporale: un caso di studio sul PM_{10}

Claudia Cappello and Sandra De Iaco and Donato Posa

Abstract Different forms of non-separability for space-time covariance functions have been recently defined in the literature, then various well-known non-separable space-time stationary covariance models are analyzed and classified according to the notion of non-separability. These results can be helpful to generate as well as to select appropriate covariance models for describing space-time data. Box-plots of sample non-separability ratios, classified for spatial lags and temporal lags, have been proposed as an appropriate diagnostic tool to detect different forms of non-separability and to support the choice of the type of non-separability which should characterize a suitable covariance model for the data. The analysis of the non-separability index for some covariance models and the space-time sample covariance function for PM_{10} data are presented.

Abstract *Recentemente, sono state definite alcune tipologie di non-separabilità, sulla base delle quali è possibile classificare i modelli di covarianza spazio-temporali. Tali risultati teorici risultano essere particolarmente rilevanti in quanto consentono di selezionare degli opportuni modelli di covarianza per la descrizione dei dati a struttura spazio-temporale. Nel presente lavoro verrà analizzato l'indice di non-separabilità per alcuni modelli di covarianza e per la covarianza empirica spazio-temporale relativa al* PM_{10}.

Key words: space-time covariance models, non-separability, environmental data

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1 Introduction

In the last years there has been a great demand for models describing the evolution of spatio-temporal processes. In this context, the selection of an appropriate class of models for the variable under study represents a priority problem with respect to the choice of a particular model of a specified class. In literature, various classes of space-time covariance functions are available. Under the convenient assumption that space and time could be treated separately, the product covariance model has represented the base to generate other parametric families of space-time covariance functions [2, 3, 9, 10]. Otherwise, various classes of non-separable space-time covariances have been constructed through different approaches by Cressie and Huang [1], Gneiting [7], Rodriguez and Diggle [12], among others. Many statistical tests for separability are based on parametric models [14, 8], likelihood ratio tests and subsampling [11] or spectral methods [13, 6] and can help to decide for a separable or a non-separable model; but they are not able to suggest the type of non separability and the appropriate covariance model for describing space-time data.
Section 2 reviews the definition of the non-separability index for a spatial-temporal covariance proposed by De Iaco and Posa [5]. Therefore, a classification of models with respect to the type of non-separability is discussed. Section 3 describes the implementation of the non-separability index in the R environment as a useful tool to help in modeling and describing the evolution of a spatio-temporal process and a case study regarding an environmental data-set, involving daily PM_{10} average concentrations measured at some monitoring stations is considered.

2 Positive and negative non-separability

Let Z be a second order stationary spatio-temporal random variable. A stationary space-time covariance function C is separable if there exist stationary, purely spatial and purely temporal correlation functions ρ_s and ρ_t, respectively, such that: $C(\mathbf{h}_s, h_t) = \sigma^2 \rho_s(\mathbf{h}_s)\rho_t(h_t) \quad \forall(\mathbf{h}_s, h_t) \in D \times T \subseteq \Re^{d+1}$, where $\sigma^2 = C(\mathbf{0}, 0)$ and $\rho_s(\mathbf{0}) = \rho_t(0) = 1$.
De Iaco and Posa [5] proposed a generalization of the two definitions of non-separability suggested by Rodriguez and Diggle [12] in order to distinguish between pointwise and uniformly positive and negative non-separability. In particular, given a spatio-temporal covariance, let $\rho(\mathbf{h}_s, h_t; \Theta)$ be the the corresponding spatio-temporal correlation function, De Iaco and Posa [5] proposed the following definition of positive and negative non separability:

$$r(\mathbf{h}_s, h_t; \Theta) = \frac{\rho(\mathbf{h}_s, h_t; \Theta)}{\rho(\mathbf{h}_s, 0)\rho(\mathbf{0}, h_t; \Theta)}. \tag{1}$$

Then, a covariance is uniformly positive non-separable if

$$r(\mathbf{h}_s, h_t; \Theta) > 1, \quad \forall(\mathbf{h}_s, h_t) \in D \times T \subseteq \Re^{d+1}, \quad (\mathbf{h}_s, h_t) \neq (\mathbf{0}, 0), \forall \Theta, \tag{2}$$

while it is uniformly negative non-separable if

$$r(\mathbf{h}_s, h_t; \Theta) < 1, \quad \forall(\mathbf{h}_s, h_t) \in D \times T \subseteq \Re^{d+1}, \quad (\mathbf{h}_s, h_t) \neq (\mathbf{0}, 0), \forall \Theta. \tag{3}$$

On the other hand, if $r(\mathbf{h}_s, h_t; \Theta) > 1$, for some $(\mathbf{h}_s, h_t; \Theta)$, the covariance function is pointwise positive non-separable at the same $(\mathbf{h}_s, h_t; \Theta)$. Alternatively, the co-

variance C is pointwise negative non-separable at $(\mathbf{h}_s, h_t; \Theta)$, if $r(\mathbf{h}_s, h_t; \Theta) < 1$ for the same $(\mathbf{h}_s, h_t; \Theta)$. As pointed out by De Iaco and Posa [5], a covariance function which is uniformly positive (negative) non-separable is also pointwise positive (negative) non-separable, but the converse is not true. According to the above definition [5], some classes of covariance models could be classified with reference to the type of non-separability:

- uniformly non separable models: the Gneiting class [7] and the class of space-time stationary covariance functions generated by positive mixtures [9] are characterized by uniformly positive non-separability, while the product-sum model [2] is characterized by a uniformly negative non-separability;
- models with different non-separability indexes: some example are given below.

The spherical metric model, whose analytic expression is given below

$$\rho(h; a_1, a_2, b) = \begin{cases} \left[1 - 1.5\dfrac{h}{b} + 0.5\left(\dfrac{h}{b}\right)^3\right], & 0 \le h \le b \\ 0, & h > b, \end{cases} \tag{4}$$

where $h = \left(a_1 \|\mathbf{h_s}\|^2 + a_2 |h_t|^2\right)^{0.5}$ and $b \in \Re_+$ is the spatio-temporal range, is non-uniformly non-separable, as shown in Fig. 1. In fact, given different combinations

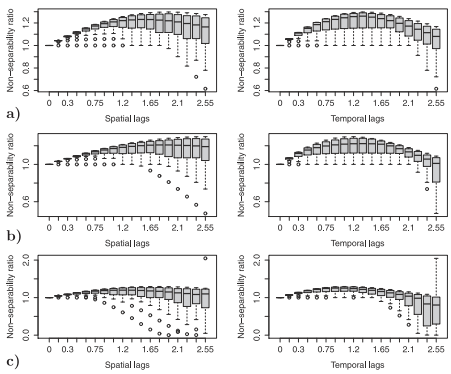

Fig. 1 box plots of non-separability ratio, defined for the spheric model (4) and classified for spatial lags and temporal lags. (a) Parameters: $a_1 = 1$, $a_1 = 2$ and $b = 5$. (b) Parameters: $a_1 = 0.2$, $a_1 = 1$ and $b = 3$. (c) Parameters: $a_1 = 0.2$, $a_1 = 0.5$ and $b = 2$.

of the parameters a_1, a_2 and b there always exist lags $(\mathbf{h}_s, h_t) \neq (\mathbf{0}, 0)$ such that $r(\mathbf{h}_s, h_t; a_1, a_2, b)$ associated to the model (4) is not always greater or less than 1. In particular, the non-separability index r is greater than 1 for small spatio-temporal lags, it becomes less than 1 when the distance h tends to the range b.
The example 4 proposed by Ma [9]

$$\rho(\mathbf{h_s}, h_t, \Theta) = \frac{log\left[1 - \theta_1\rho_s(\mathbf{h}_s) - \theta_2\rho_t(h_t) - \theta_{12}\rho_s(\mathbf{h}_s)\rho_t(h_t)\right]}{log\theta_3} \tag{5}$$

where $\theta_3 = 1 - (\theta_1 + \theta_2 + \theta_{12})$ and θ_{12} are non-negative constants such that $0 < \theta_1 + \theta_2 + \theta_{12} < 1$, is non-uniformly non-separable, that is the ratio r is greater or less than 1, depending on the lags and/or the parameter of the model (Fig. 2-a)). However,

the class of covariance functions proposed by Ma [9] is able to describe uniformly positive and negative non-separability, as shown in Fig. 2-b). The class of integrated

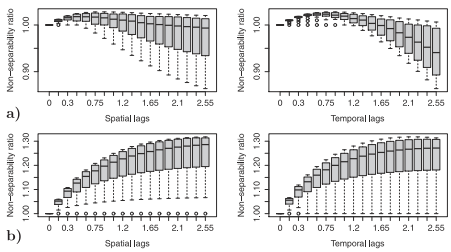

Fig. 2 box plots of non-separability ratio, defined for a mixture model proposed by Ma (5) and classified for spatial lags and temporal lags. (a) Parameters: $a_1 = 1$, $a_1 = 2$, $\theta_1 = 0.1$, $\theta_2 = 0.3$ and $\theta_{12} = 0.2$. (b) Parameters: $a_1 = 2$, $a_1 = 2$, $\theta_1 = 0.1$, $\theta_2 = 0.2$ and $\theta_{12} = 0.5$

models, proposed by De Iaco et al. [3] is flexible enough to handle either uniformly positive and negative non-separability or non-uniform non-separability, depending on the lags and/or to the parameters of the chosen models. In particular, consider the following integrated product-sum model:

$$\rho(\mathbf{h}_s,h_t,\Theta)=\int_0^\infty\left[k_1e^{-x\|\mathbf{h_s}\|^\alpha/b}e^{-x|h_t|^\delta/c}+k_2e^{-x\|\mathbf{h_s}\|^\alpha/b}+k_3e^{-x|h_t|^\delta/c}\right]\frac{\beta^{n+1}}{\tau(n+1)}x^ne^{-\beta x}dx$$
$$=k_1\frac{\beta^{n+1}}{\left(\frac{\|\mathbf{h_s}\|^\alpha}{b}+\frac{|h_t|^\delta}{c}+\beta\right)^{n+1}}+k_2\frac{\beta^{n+1}}{\left(\frac{\|\mathbf{h_s}\|^\alpha}{b}+\beta\right)^{n+1}}+k_3\frac{\beta^{n+1}}{\left(\frac{|h_t|^\delta}{c}+\beta\right)^{n+1}} \qquad (6)$$

where $\Theta=(b,c,\alpha,\delta,k_1,k_2,k_3,\beta,n)$ is the parameters vector.
Let $\Theta=(1,1,1,1,0.4,0.3,0.3,2,2)$ the integrated product-sum model describes space-time covariances that are uniformly negative non-separable (Fig. 3-a)); on the other hand, let $\Theta=(1,1,2,2,0.7,0,0.3,2,2)$ the integrated product-sum model describes space-time covariances that are uniformly positive non-separable (Fig. 3-b)). Finally, if $\Theta=(1,1,1,1,0.6,0.1,0.3,1,1)$ the integrated product-sum model

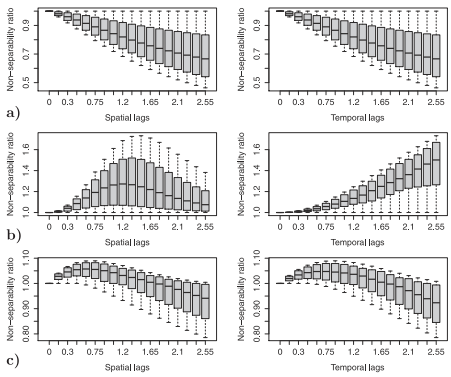

Fig. 3 box plots of non-separability ratio, defined for the integrated product-sum model (6) and classified for spatial lags and temporal lags.

describes space-time covariances that are non-uniformly non-separable (Fig. 3-c)). The class of models proposed by Rodriguez and Diggle [12] is given below

$$C(\mathbf{h}_s, h_t, \Theta) = \frac{\sigma^2}{2}\left[\rho_{s,1}(\mathbf{h}_s;\theta_1)\rho_{t,1}(h_t;\phi_1) + \rho_{s,2}(\mathbf{h}_s;\theta_2)\rho_{t,2}(h_t;\phi_2)\right] \tag{7}$$

where $\rho_{s,1}(\mathbf{h}_s;\theta_1), \rho_{s,2}(\mathbf{h}_s;\theta_2), \rho_{t,1}(h_t;\phi_1), \rho_{t,2}(h_t;\phi_2)$ are, respectively, two non-negative and integrable spatial correlation functions and two non-negative and integrable temporal correlation functions. Note that the above class of covariance functions could be considered as a special case of integrated product models.
If $\rho_{s,1}(\mathbf{h}_s, a_{s_1}) = e^{-a_{s_1}\|\mathbf{h_s}\|}$ and $\rho_{s,2}(\mathbf{h}_s, a_{s_2}) = e^{-a_{s_2}\|\mathbf{h_s}\|}$, and similarly $\rho_{t,1}$ and $\rho_{t,2}$ are exponential models with parameters a_{t_1} and a_{t_2}, then the Rodriguez and Diggle model is uniformly positive non-separable when $a_{s_1} > a_{s_2}$ and $a_{t_1} > a_{t_2}$ (Fig. 4-a)), whereas they are uniformly negative non-separable when $a_{s_1} < a_{s_2}$ and $a_{t_1} > a_{t_2}$ (and viceversa), Fig. 4-b). Otherwise, if $\rho_{s,1}(\mathbf{h}_s, a_{s_1}) = e^{-a_{s_1}\|\mathbf{h_s}\|^2}$ and $\rho_{s,2}(\mathbf{h}_s, a_{s_2}) = e^{-a_{s_2}\|\mathbf{h_s}\|}$, and $\rho_{t,1}$ and $\rho_{t,2}$ are exponential and Gaussian models, respectively, with parameters a_{t_1} and a_{t_2}, then they are non uniformly non-separable (Fig. 4-c),-d)).

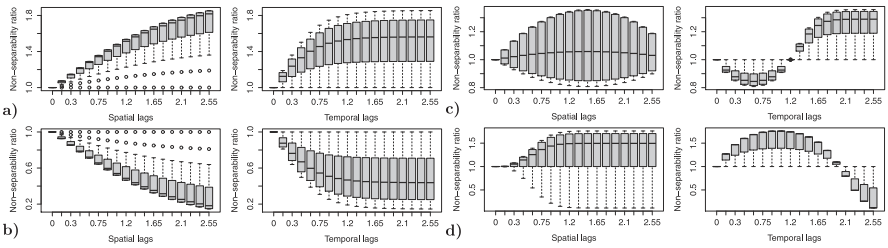

Fig. 4 box plots of non-separability ratio, defined for the Rodriguez and Diggle model (7) and classified for spatial lags and temporal lags.

3 Case study

In this paper, the new function called `sep_index`, defined for determining non-separability index (1) in the R environment, has been applied in order to analyze the space-time correlation structure of the daily PM_{10} averages, observed at some monitoring stations, from 1998 to 2009.
Structural analysis and non-separability inspection could be performed in the R environment (with packages `spacetime` and `gstat`) through the following steps: 1) create a spatio-temporal object to record the data set; 2) determined sample spatio-temporal variogram surface; 3) inspect marginal variograms (`vario_marg`); 4) compute sample spatio-temporal covariance surface; 5) compute the empirical non-separability index (`sep_index`). Note that the new function called `vario_marg` has been properly developed in order to compute, plot and model marginal variograms. The new function, named `sep_index` requires some parameters to be set: the number of spatial lags (`ns`), the number of temporal lags (`nt`), the matrix in which the spatio-temporal covariogram values (`cov`) are stored and the value of the global sill (`globalSill`). The function `sep_index` returns the purely spatial and purely temporal sample covariances matrix, empirical non-separability index ratio and box-plots of sample non-separability ratios, classified for spatial lags and temporal lags. For the environmental data set under study, sample non-separability

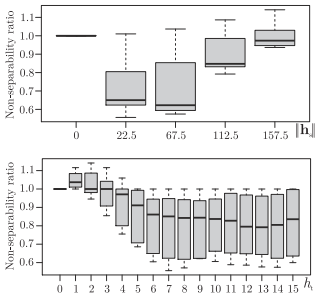

Fig. 5 box-plots of sample non-separability ratio, computed for daily averages PM_{10} concentrations and classified for (a) spatial lags and (b) temporal lags

index is less than 1 for all $\mathbf{h}_s, h_t$ (Fig. 5). Hence, it should be suitable to select a covariance model characterized by uniformly negative non-separability, such as the integrated product-sum model (6) and the Rodriguez and Diggle (7) for appropriate choices of the coefficients and the marginals.

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