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**SDATIA STATISTICS** 

## A closer look at the spatial exponential matrix specification



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#### a b s t r a c t

In this paper we analyze the partial and marginal covariance structures of the spatial model with the covariance structure based on a exponential matrix specification. We show that this model presents a puzzling behavior for many types of geographical neighborhood graphs, from the simplest to the most complex. In particular, we show that for this model it is usual to have opposite signs for the marginal and conditional correlations between two areas. We show these results through experimental examples and analytical demonstrations.

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#### **1. Introduction**

Suppose we have a region *R* partitioned into *n* disjoint areas  $A_1, A_2, \ldots, A_n$  such that  $\cup_{i=1}^n A_i = R$ . The data observed in each of these areas are, typically, counts, sums or some type of aggregated value of characteristics associated with the each of these units. In order to introduce the spatial dependence between them, we need to define a neighborhood structure according to the geographical arrangement of these areas. Once defined the neighborhood structure, we specify models reflecting the geographical location of the data. One recurrent approach relies on ideas from autoregressive time series models. A popular model that include this type of structure is the Simultaneous Autoregressive (SAR) model [\(Whitle,](#page--1-0) [1954\)](#page--1-0). The SAR model is specified by a set of regression equations in which the dependent variable is the observation in a particular area and the explanatory variables are

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the observations on their neighbors. This system of equations is solved simultaneously inducing a multivariate normal distribution.

Let  $y_i$  be a value observed in area  $A_i$ . The SAR model is determined by the simultaneous solution of the set of equations given by:

<span id="page-1-0"></span>
$$
Y_i = \mu_i + \sum_{j=1}^n s_{ij} (Y_j - \mu_j) + \epsilon_i \quad \text{for } i = 1, ..., n,
$$
 (1)

where  $\epsilon_i$  are i.i.d. normally distributed with variance  $\sigma^2,~\mu_i=E(Y_i)$ , and  $s_{ij}$  are parameter-dependent constants with  $s_{ii} = 0$ . If  $Y = (Y_1, Y_2, \ldots, Y_n)$ , then the set of equations [\(1\)](#page-1-0) leads to a multivariate normal distribution for **Y**:

$$
\mathbf{Y} \sim N\left(\boldsymbol{\mu}, \sigma^2(\mathbf{I}-\mathbf{S})^{-1}(\mathbf{I}-\mathbf{S}^T)\right),
$$

where  $\mu = (\mu_1, \mu_2, \dots, \mu_n)$  and the matrix **S** is composed by the constants  $s_{ii}$  constrained in such a way as to guarantee the existence of  $(\mathbf{I}-\mathbf{S})^{-1}.$ 

The maximum likelihood estimator of the unknown parameters, including the parameter dependent matrix, is typically hard to obtain due to the constrained optimization and the need to deal with the determinant of the covariance matrix. [LeSage](#page--1-1) [and](#page--1-1) [Kelley](#page--1-1) [Pace](#page--1-1) [\(2007\)](#page--1-1) present a new spatial model that bypass these numerical problems. This is a particular case of the proposal made by [Chiu](#page--1-2) [et al.](#page--1-2) [\(1996\)](#page--1-2) where general covariance matrices are expressed as the exponential function applied to a certain matrix. A major advantage of this definition is that it guarantees that the covariance matrix is always positive definite. Thus, it becomes unnecessary to put constraints on the parameter space during the estimation procedure to ensure that this property is satisfied. Another advantage is the simple way to obtain the precision matrix.

However, as we show in this paper, the exponential matrix covariance model has a major disadvantage when used in the spatial context. Mainly, this model is not flexible enough to incorporate many covariance patterns that one would expect to find in practice. The model is restricted to covariance patterns that have, in fact, non-intuitive aspects. The main point is that using this approach, in most practical situations, it will lead to opposite signs for the marginal and the partial correlations between pairs of neighboring areas. This limitation implies in an undesirable restrictive behavior for the stochastic structure of the data and therefore requires careful justification for its use. In Section [2,](#page-1-1) we study the properties of this exponential covariance matrix in detail starting by describing the model proposed by [LeSage](#page--1-1) [and](#page--1-1) [Kelley](#page--1-1) [Pace](#page--1-1) [\(2007\)](#page--1-1). Consider the partial correlation Cor(*Yi*, *Y<sup>j</sup>* |**Y**−*ij*), given all the other variables **Y**−*ij* in the map. We prove in Section [3](#page--1-3) that, for even-order neighboring pairs, Cor(*Yi*, *Y<sup>j</sup>* |**Y**−*ij*) has the opposite sign as the marginal Cor(*Yi*, *Yj*), irrespective of the value of the coefficients in the model. In Section [4,](#page--1-4) we show that this behavior is non-intuitive and it is not allowed in the usual time series models. In irregular lattices, as those used in geographical data analysis, we showed in Section [5](#page--1-5) that the non-intuitive sign change behavior of second-order neighbors is common although not guaranteed. In fact, we show that this happens for certain range of the exponential matrix parameters. Using matrix derivatives, we demonstrate that as the spatial correlation parameter increases, this puzzling behavior is intensified. More disconcerting, we show that, even for firstorder neighboring areas in real maps, we can easily generate different signs for marginal and partial correlations. In Section [7,](#page--1-6) we discuss the consequences of this behavior and present our conclusions.

#### <span id="page-1-1"></span>**2. Model definition**

To guarantee that the normal distribution induced by the set of simultaneous equations [\(1\)](#page-1-0) is proper, the matrix (**I** − **S**) must be of full rank. One possibility to ensure this property is to set  $S = \rho D$  and put restrictions on the space where the parameter  $\rho$  is defined. The matrix **D** can be specified in various ways. The two most common approaches are the following. In the first one, denoted by **W**, we define a binary matrix: **W***ij* receives value 1 if the areas *i* and *j* are neighbors, and zero otherwise. Additionally,  $W_{ii} = 0$ . Another commonly used alternative is to define the matrix **D** 

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