# Another close look at the spatial structure of CAR and SAR models

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#### 8 Abstract

- $_{\rm 9}$   $\,$   $\,$  The conditional autoregressive model (CAR) and the simultaneous autoregressive
- model (SAR) are widely used to model the spatial correlation of lattice data. Several
- 11 authors have pointed out impractical or counterintuitive consequences produced by
- these models for the covariance matrix. This paper clarifies many of these puzzling
- 13 results. We show that the neighborhood graph structure, synthesized in eigenvalues
- 14 and eigenvectors structure of a matrix associated with the adjacency matrix, de-
- 15 termines most of the apparently anomalous behavior. We illustrate our conclusions
- 16 with regular and irregular lattices including lines, grids and lattices based on real
- 17 maps.
- 18 Key words: Spatial interaction, Lattice data, Spatial autoregression
- 19 PACS: code, code

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#### 20 1 Introduction

- Lattice data refer to statistical data observed at spatial locations or areas in a given geographical region. It is common to assume that observations at sites near each other tend to have similar values. The Conditional Autoregressive (CAR) and the Simultaneous Autoregresive (SAR) models are widely used to analyze these lattice data. The SAR model is preferred in likelihood inference, while the CAR model is more common in Bayesian inference as a prior distribution for spatially structured random effects.
- Despite their popularity, these models bring uneasy consequences for the implied correlation structure of the variables. Several authors have pointed out
  that the SAR and CAR models yield non constant variances at each site as
  well as unequal covariances between regions separated by the same number of
  neighbors (Haining, 1990, page 82; Besag and Kooperberg, 1995).
- Wall (2004) extensively studied the covariance structure entailed by these models. She found that the implied correlation between a pair of neighboring areas is negatively associated with the number of neighbors of each region. However, she also showed that this relationship is not simple and much variability remains unexplained. For example, considering the three neighboring US states Missouri, Arkansas, and Tennessee, she showed that, although Missouri and Tennessee have the same neighboring structure, their correlation with Arkansas differs. She also showed that sites with equal number of neighbors can have different variances.

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In addition to these uncomfortable results, Wall (2004) pointed out a series of puzzling results from these two spatial models. One of them is that correlations between areas switch their ranks depending on  $\rho$ , a spatial dependence parameter. Suppose that a pair (i,j) of sites are more correlated than another pair (k,l) when  $\rho=0.5$ . It is not uncommon that when  $\rho=0.7$ , the pair (k,l) becomes more correlated than (i,j). One would expect, perhaps naively, that the order should be the same, irrespective of the spatial dependence parameter value. Even more puzzling are the results concerning negative values for  $\rho$ . She found that when  $\rho$  is negative, correlations between the neighboring areas are also negative but, as  $\rho$  decreases further, some pairs of areas start to be positively correlated, even approaching +1 at times.

Wall (2004) concluded that the implied spatial correlation between the different sites using the SAR and CAR models does not seem to follow an intuitive or practical scheme and she called for more research to be carried out to clarify these problems. This is the main purpose of this paper. We explain the apparently counterintuitive or impractical consequences of the model specification by using the complete neighborhood graph structure, not only the immediate neighborhood. In accounting for the complete neighborhood structure, we see that a crucial role is played by the second largest eigenvalue modulus of the neighborhood matrix used in the SAR and CAR models. We use a simple matrix algebra identity to write the covariance matrices of the SAR and CAR models as a matrix power series. This enables us to express the correlation between any two pairs of areas i and j as an infinite series with exponential decay given by the spatial dependence parameter  $\rho$ . Moreover, the k-th term coefficient of this series is proportional to a weighted sum of the different paths to move from area i to area j in k steps. In Section 2, the CAR and SAR models are defined and we illustrate the implied consequences for the covariance structure by means of an example with the US continental states. Section 3 reviews the linear algebra definitions and results relevant for this paper and Section 4 shows how many of the puzzling results can be understood. Conclusions are presented in Section 5.

#### 2 The SAR and CAR models

Let a region D be partitioned into n areas  $\{A_1, \ldots, A_n\}$  such that  $D = A_1 \cup \ldots \cup A_n$  and  $A_i \cap A_j = \text{for all } i \neq j$ . Let  $y_i$  be a random variable measured at area i and  $\mathbf{y} = (y_1, \ldots, y_n)^t$ . We denote by  $\mathbf{y}_{-i}$  the (n-1)-dimensional vector without the i-th coordinate of  $\mathbf{y}$ . The conditional autoregressive model (CAR) is given by a set of n conditional distributions

$$y_i | \boldsymbol{y}_{-i} \sim N\left(\mu_i + \sum_{j=1}^n c_{ij}(y_j - \mu_j), \kappa_i^2\right)$$
 (1)

where  $c_{ii} = 0$  and  $\kappa_i^2 > 0$  for i = 1, ..., n. It is not any set of n conditional distributions that determine uniquely a joint distribution for the vector  $\boldsymbol{y}$ . However, a very popular choice in spatial studies for the constants  $c_{ij}$  and  $\kappa_i$  defines a valid joint model, and we adopt this choice in the rest of this paper.

The choice of the  $n \times n$  matrix  $\boldsymbol{C} = (c_{ij})$  is related to the degree of spatial proximity between areas i and j. Let  $\boldsymbol{A} = (a_{ij})$  be an  $n \times n$  binary neighborhood matrix such that  $a_{ij} = 1$  if, and only if, areas i and j are neighbors (denoted by  $i \sim j$ ). We let  $a_{ii} = 0$ . Define  $\boldsymbol{W} = (w_{ij})$  such that  $w_{ij} = a_{ij}/a_i$ . where  $a_i = \sum_j a_{ij} = d_i$ , the number of neighboring areas of region i. Finally, define  $\boldsymbol{C} = \rho_c \boldsymbol{W}$  and  $\kappa_i = \sigma_c^2/d_i$ . Under a restriction on the value of  $\rho_c$ , the

CAR model (1) with these options defines a valid joint distribution for the vector  $\boldsymbol{y}$  given by a multivariate normal distribution:

$$\mathbf{y} \sim N_n \left( \boldsymbol{\mu}, (\boldsymbol{I} - \rho_c \boldsymbol{W})^{-1} \boldsymbol{K} \right)$$
 (2)

where  $\boldsymbol{\mu} = (\mu_1, \dots, \mu_n)'$ ,  $\boldsymbol{I}$  is the identity matrix and  $\boldsymbol{K}$  is the diagonal matrix diag $(\kappa_1, \dots, \kappa_n)$  which is equal to  $\sigma_c^2 \operatorname{diag}(d_1^{-1}, \dots, d_n^{-1})$ . The restriction on  $\rho_c$  is necessary to ensure that  $(\boldsymbol{I} - \rho_c \boldsymbol{W})^{-1} \boldsymbol{K}$  is positive definite and it suffices to take  $\rho_c$  such that  $\rho_c$  is between  $1/\min_i \lambda_i$  and  $1/\max_i \lambda_i$  where  $\lambda_i$ ,  $i = 1, \dots, n$ , are the eigenvalues of  $\boldsymbol{W}$  (Haining, 1990, page 82).

This choice also implies that (1) reduces to

$$y_i|\boldsymbol{y}_{-i} \sim N\left(\mu_i + \rho_c \overline{(y-\mu)}_i, \sigma_c^2/d_i\right)$$
(3)

where  $\overline{(y-\mu)}_i = \sum_j w_{ij}(y_j - \mu_j)$  is the average of the deviations  $y_j - \mu_j$  among  $j \sim i$ , i.e. among the neighboring areas of i.

The SAR model is defined by n simultaneous equations

$$y_i = \mu_i + \sum_{j=1}^n s_{ij} (y_j - \mu_j) + \epsilon_i$$
 (4)

where  $\epsilon = (\epsilon_1, ..., \epsilon_n)' \sim N(0, \mathbf{\Lambda})$  with  $\mathbf{\Lambda}$  diagonal,  $E(y_i) = \mu_i$ , and  $s_{ij}$  are known constants with  $s_{ii} = 0, i = 1, ..., n$ . This model is *simultaneous* because the random variables are simultaneously determined by the n equations in 4. Provided that the inverse of the matrix  $I_n - S$  exists, the distribution of  $\mathbf{y} = (y_1, ..., y_n)'$  is

$$y \sim N(\mu, (I_n - S)^{-1} \Lambda (I_n - S)^{-1'}),$$
 (5)

where  $S_{ij} = s_{ij}$ . A popular choice for  $\mathbf{S}$  is to take  $\mathbf{S} = \rho_s \mathbf{W}$ , where  $\rho_s \in$  (-1, 1). Following Wall (2004), we will constrain  $\rho_s$  to the same interval as  $\rho_c$  in order to allow for comparisons between the models.

With these choices for the SAR and CAR model, the correlation matrix entries are functions of only  $\boldsymbol{W}$  and  $\rho_c$  or  $\rho_s$ . For example, for the CAR model, we have

$$\operatorname{Cor}(i,j) = \frac{\sigma_c^2 (I - \rho_c \boldsymbol{W})_{ij}^{-1} d_j^{-1}}{\sqrt{\sigma_c^2 (I - \rho_c \boldsymbol{W})_{ii}^{-1} d_i^{-1}} \sqrt{\sigma_c^2 (I - \rho_c \boldsymbol{W})_{jj}^{-1} d_j^{-1}}},$$

and  $\sigma_c^2$  is canceled out.

## 118 2.1 The puzzling results

We summarize the main puzzling results concerning the correlations implied by the SAR and CAR models and described by Wall (2004). She used the United 120 States map to illustrate the implications that the CAR and SAR models entail for the covariance between pairs of areas. Consider the graph composed by the 122 48 contiguous continental states. Two states i and j are connected by an edge 123 (meaning that  $w_{ij} > 0$ ) if they share borders. This graph is in Figure 2.1, 124 with the underlying US map. The upper right plot in Figure 1 shows the correlations Cor(i, j) between pairs of neighboring states by the number of neighbors. Every pair (i, j) of neighboring areas contribute two points in this 127 plot depending on each area's number of neighbors, the pair  $(d_i, \text{Cor}(i, j))$  and 128 the pair  $(d_i, \operatorname{Cor}(i, j))$ . We can see that, for a given number of neighbors, there is a large variation in the correlations.

The lower row of plots in Figure 2.1 shows how the correlations Cor(i, j) varies

with the spatial dependence parameter  $\rho$ . Each line represents the correlation between two neighboring areas and the horizontal axis corresponds to the spatial dependence parameter  $\rho_s$  of the SAR model (left hand side plot), or  $\rho_c$  for the CAR model (right hand side plot). Based on the eigenvalues of  $\boldsymbol{W}$ for the US lattice, a restriction for the spatial parameter space (-1.392, 1).

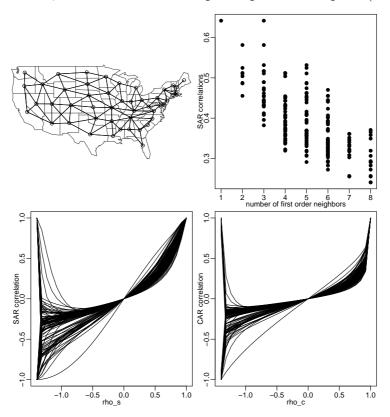


Fig. 1. The graph of USA states by neighborhod, SAR correlations implied by number o neighbors if  $\rho_s = 0.6$  and the correlations implied by SAR and CAR models for all possible  $\rho_s$  and  $\rho_c$  values

Most of the puzzling results appear in these plots. We can see that lines cross each other as  $\rho$  varies, irrespective of the model adopted. This means that, if we increase the spatial correlations between all pairs of areas by increasing  $\rho$ , states which are less correlated than others can become more correlated after varying  $\rho$ . For example, when  $\rho_c = 0.49$ , the correlation between Alabama and Georgia and Florida is 0.1993 while the correlation between Alabama and Georgia

is 0.1561. However, when  $\rho_c = 0.97$ , the correlation between Alabama and Florida is 0.6311, smaller than the correlation between Alabama and Georgia, which is equal to 0.6490. This seems odd as it means that the effect of changing  $\rho$  is not uniquely defined.

Consider the behavior of Cor(i, j) when  $\rho$  approaches its lower bound -1.392. the pairwise correlations approach either -1 or +1. The latter limit value is counter-intuitive: some pairs tend to be perfectly positively correlated when we expect they to be the opposite of their neighboring values according to the SAR or CAR models.

Some results are reassuring. The correlations increase monotonically with  $\rho$  when the spatial dependence parameter is positive. However, the range of the correlations depends on the value of  $\rho$ . For instance, when  $\rho_s=0.1$ , correlations between neighboring states vary between 0.026 and 0.115, while this variation lies between 0.241 and 0.642 when  $\rho_s=0.6$ .

# <sup>157</sup> 3 Some preliminary definitions and results

To explain the puzzling consequences, we use linear algebra and graph theory results.

## $_{160}$ 3.1 Random graphs and the matrix W

The W matrix can be seen as the transition matrix of a Markov chain defined on a graph. Assume that n nodes or vertices, represented by the areas  $A_i$ , are connected by undirected edges such that there is an edge between areas i and j if  $w_{ij} \neq 0$ . Define a discrete-time and finite Markov chain with transition matrix given by W. That is, if a particle is in one vertex i at time t, it moves to a different vertex in the next moment choosing among the neighbors of  $A_i$ with equal probability. These type of Markov models are called random walks on graphs (Brémaud, 1999, page 214), or random graph, for short.  $W^k$  is the transition matrix for the chain movements in k steps.

The random walk on the neighborhood graph converges to a unique stationary distribution if the Markov chain defined by  $\boldsymbol{W}$  is ergodic and aperiodic. For this, the graph must be connected, i.e., from each node there exists a path of edges connecting successive nodes until any other arbitrarily chosen node is reached. If  $\boldsymbol{W}$  is the normalized adjacency matrix of an undirected graph  $\boldsymbol{G}$ , then the stationary distribution of the Markov chain defined by  $\boldsymbol{W}$  is given by  $\boldsymbol{\pi} = (\pi_1, ..., \pi_n)$  where  $\pi_i = d_i/D$ , where  $d_i$  is the number of neighbooring areas of i and  $D = \sum_i d_i$  (see Brémaud, 1999, page 214).

This implies that the power  $W^k$  converge to a matrix composed by identical rows, all of them equal to the stationary distribution vector  $\pi$ . That is,  $W^k_{ij} \to d_j/D$ , as  $k \to \infty$ . The convergence to this stationary distribution is geometric, with relative speed proportional to the second-largest eigenvalue modulus. This result is known as the Perron-Fröbenius theorem (Brémaud, 1999, page 157) and it is important for our development. It can be shown that the eigenvalue of W with the largest modulus has multiplicity 1 and it is  $\lambda = 1$ . Let  $\lambda_2, \ldots, \lambda_n$  be the other eigenvalues of W ordered in a such a way that

$$\lambda_1 = 1 \ge |\lambda_2| > \ldots \ge |\lambda_n|.$$

Let  $m_2$  be the multiplicity of  $\lambda_2$  and  $\mathbf{1}=(1,\ldots,1)^t$ . Then, the Perron-Fröbenius theorem proves that

190 
$$\mathbf{W}^k = \mathbf{1} \; \boldsymbol{\pi}^t + O(k^{m_2 - 1} |\lambda_2|^k) \;,$$

where k is a positive constant. In particular, if  $|\lambda_2| > |\lambda_3|$  then  $m_2 = 1$  and the convergence speed decays exponentially with the second largest eigenvalue modulus  $|\lambda_2|$ .

#### 3.2 A matrix identity

There is a matrix identity which is fundamental to understanding the behavior of the correlations implied by the models and described in Section 2. If M is a square matrix such that each entry of the matrix  $M^k$  goes to zero as k increases, then the inverse  $(I - M)^{-1}$  exists and is given by

$$(I - M)^{-1} = I + M + M^{2} + M^{3} + \dots$$
 (6)

(see Iosifescu, 1980, page 45). Take  $\boldsymbol{M} = \rho \boldsymbol{W}$  where  $|\rho| < 1$ . Since  $0 \leq \boldsymbol{W}_{ij}^k \leq$  1 for all i, j and for all integer k, we can write

$$(I - \rho \mathbf{W})^{-1} = I + \rho \mathbf{W} + \rho^2 \mathbf{W}^2 + \rho^3 \mathbf{W}^3 + \dots$$
 (7)

# 3.3 The powers of the $oldsymbol{W}$ matrix

If  $[\mathbf{W}^k]_{ij} > 0$ , then the probability of going from i to j in k steps in the random graph is positive. This means that there exists at least one sequence of k edges connecting nodes such that the initial and final nodes are i and j,

respectively. Let us call such a path of a k-th order path between areas i and j. In fact, the value of  $[\mathbf{W}^k]_{ij}$  is a weighted sum of all the k-th order paths between i and j. For example,  $[\mathbf{W}^2]_{ij}$  is given by

$$[\mathbf{W}^2]_{ij} = \sum_{k=1}^n W_{ik} W_{kj} = \sum_{k=1}^n \frac{a_{ik}}{d_i} \frac{a_{kj}}{d_k} = \frac{1}{d_i} \sum_{k=1}^n \frac{a_{ik} a_{kj}}{d_k} . \tag{8}$$

The binary product  $a_{ik}a_{kj}$  is equal to 1 only if k connects both i and j.

Therefore,  $[\mathbf{W}^2]_{ij}$  is proportional to a weighted sum of all second-order paths  $i \to k \to j$ . Each path contributes a fraction inversely proportional to the number  $d_k$  of neighbors the intervening area k has. The more connected k is, the smaller the contribution of the path  $i \to k \to j$  to  $[\mathbf{W}^2]_{ij}$ . Note that  $[\mathbf{W}^2]_{ii} > 0$  because there is at least one path of the type  $i \to k \to i$  since each area has at least one neighbor.

Similarly,  $[\boldsymbol{W}^3]_{ij}$  is given by

$$[\boldsymbol{W}^{3}]_{ij} = \sum_{l=1}^{n} [\boldsymbol{W}^{2}]_{il} w_{lj} = \frac{1}{d_{i}} \sum_{l=1}^{n} \sum_{k=1}^{n} \frac{a_{ik} a_{kl} a_{lj}}{d_{k} d_{l}}.$$
 (9)

Each path  $i \to k \to l \to j$  is inversely weighted by how dense is the neighborhood graph at k and l. Note that paths such as  $i \to j \to i \to j$  are also counted.

## 223 4 Revisiting the puzzling results

Putting together the results of Section 3, for  $|\rho| < 1$ , we can write

$$[(\mathbf{I} - \rho \mathbf{W})^{-1}]_{ij} = [\mathbf{I}]_{ij} + \rho [\mathbf{W}]_{ij} + \rho^2 [\mathbf{W}^2]_{ij} + \rho^3 [\mathbf{W}^3]_{ij} + \dots$$
 (10)

As long as  $|\rho| < 1$ , the correlation between i

Since the k-th coefficient  $[\boldsymbol{W}^k]_{ij}$  can be interpreted as a probability, it lies between 0 and 1. Furthermore,  $[\boldsymbol{W}^k]_{ij}$  approaches the limit  $d_j/D$  for all iand the speed of this convergence, for all i and j, is determined by the second largest eigenvalue modulus of  $\boldsymbol{W}$ . This means that, with a good approximation and for some value k, we can write

$$[(\boldsymbol{I} - \rho \boldsymbol{W})^{-1}]_{ij} \approx [\boldsymbol{I}]_{ij} + \rho [\boldsymbol{W}]_{ij} + \dots + \rho^{k-1} [\boldsymbol{W}^{k-1}]_{ij} + \frac{d_j \rho^k}{D(1-\rho)}$$

$$\approx [\boldsymbol{I}]_{ij} + \rho [\boldsymbol{W}]_{ij} + \dots + \rho^{k-1} [\boldsymbol{W}^{k-1}]_{ij}$$

$$(12)$$

With these facts, the results are less puzzling and easier to understand. Basically, when we naively try to understand the covariance structure focusing only on the first-order neighborhood structure, we are doomed from the start. For instance, if the third degree approximation in (12) suffices, we have the CAR model covariance between areas i and j, ieqj, given approximately by  $\frac{\kappa^2}{d_j} \left( \frac{\rho a_{ij}}{d_i} + \frac{\rho^2}{d_i} \sum_{k=1}^n \frac{a_{ik} a_{kj}}{d_k} + \frac{\rho^3}{d_i} \sum_{k=1}^n \sum_{k=1}^n \frac{a_{ik} a_{kl} a_{lj}}{d_l d_k} \right)$ 

Ignoring the neighborhood structure geographically more distant than the first order will produce a crude approximation to the true correlation coefficient. Giving due consideration to the longer paths from i to j, though with ever decreasing weight, we find the results described by Wall (2004) to be much less puzzling, as we discuss next.

## <sup>243</sup> 4.1 The CAR model with $\rho_c > 0$

First, let us consider the CAR model and  $\rho_c > 0$ . Then, (10) shows that the correlation must increase monotonically with  $\rho_c$ , since all the coefficients in

that series expansion are nonnegative. This is one of the empirical results from Wall (2004). Although it is what one expects intuitively, now we understand the underlying reason for this monotone increase of Cor(i, j).

However, correlations of different pairs can increase at different rates. This is because the series expansion coefficients in (10) are pair-specific. In fact, the derivative of  $[(I - \rho W)^{-1}]_{ij}$  is equal to

$$\frac{\partial}{\partial \rho} [(\boldsymbol{I} - \rho \boldsymbol{W})^{-1}]_{ij} = [\boldsymbol{W}]_{ij} + 2\rho [\boldsymbol{W}^2]_{ij} + 3\rho^2 [\boldsymbol{W}^3]_{ij} + \dots$$
(13)

This implies that, for  $\rho \in (0,1)$ , we have an increasing derivative with  $\rho$ . If  $\rho$  is not too close to 1, the rate of increase of this derivative depends mostly on the second-order neighborhood  $[\boldsymbol{W}^2]_{ij}$ .

Different pairs can exchange their relative positions as  $\rho_c > 0$  increases and it is clear now why and when this happens. The derivative on (13) depends of the specific pair i, j under consideration. For example, assuming that the second degree polynomial approximation in (12) is good enough, then

$$\frac{\partial}{\partial \rho} [(\boldsymbol{I} - \rho \boldsymbol{W})^{-1}]_{ij} \approx [\boldsymbol{W}]_{ij} + 2\rho [\boldsymbol{W}^2]_{ij}$$
(14)

Therefore, the larger  $\rho_c$ , the greater the positive contribution of the secondorder neighborhoods. Hence, when  $\rho_c$  is small, a pair (i,j) can have a small correlation that may increases faster than the correlation in other areas simply because its second order coefficient  $[\boldsymbol{W}^2]_{ij}$  is relatively large.

This is the explanation for the apparently strange behavior of the switching ranks between the correlations of Alabama and Florida and Alabama and Georgia. We use Table 1 to illustrate our arguments focusing on the CAR

Table 1 Values of the entries of  $\boldsymbol{W}^k$ ,  $\rho^k \boldsymbol{W}^k$ , and the cumulative sum  $\sum_{j=0}^k \rho^j \boldsymbol{W}^j$  for the pairs of neighboring states (Alabama, Florida) and (Alabama, Florida). We consider the values  $\rho = 0.97$  and  $\rho = 0.49$ .

k	1	2	3	4	5	10	30	50	100		
Alabama and Florida, $\rho_c=0.97$											
$oldsymbol{W}^k$	0.2500	0.0500	0.0984	0.0498	0.0588	0.0317	0.0127	0.0100	0.0094		
$ ho^k oldsymbol{W}^k$	0.2425	0.0470	0.0898	0.0441	0.0505	0.0233	0.0051	0.0022	0.0004		
CumSum	0.2425	0.2895	0.3794	0.4235	0.4740	0.6246	0.8345	0.8997	0.9526		
Alabama and Georgia, $\rho_c=0.97$											
$oldsymbol{W}^k$	0.2500	0.1562	0.1516	0.1333	0.1179	0.0754	0.0312	0.0249	0.0234		
$ ho^k oldsymbol{W}^k$	0.2425	0.1470	0.1383	0.1180	0.1012	0.0556	0.0125	0.0054	0.0011		
CumSum	0.2425	0.3895	0.5278	0.6458	0.7470	1.1026	1.6092	1.7711	1.9030		
Alabama and Florida, $\rho_c = 0.49$											
$\rho^k W^k$	0.1225	0.0120	0.0116	0.0029	0.0017	0.0000	0.0000	0.0000	0.0000		
CumSum	0.1225	0.1345	0.1461	0.1490	0.1506	0.1517	0.1517	0.1517	0.1517		
Alabama and Georgia, $\rho_c = 0.49$											
$ ho^k oldsymbol{W}^k$	0.1225	0.0375	0.0178	0.0077	0.0033	0.0001	0.0000	0.0000	0.0000		
CumSum	0.1225	0.1600	0.1778	0.1855	0.1889	0.1915	0.1915	0.1915	0.1915		

model with  $\rho_c=0.97$  and  $\rho_c=0.49$ . For Alabama and Florida,

[
$$(\boldsymbol{I} - \rho \boldsymbol{W})^{-1}$$
]<sub>Al, Fl</sub>  $\approx 0.25\rho + 0.05\rho^2 + 0.10\rho^3 + 0.05\rho^4 + \dots$ 

vhile, for Alabama and Georgia, we have

$$[(\boldsymbol{I} - \rho \boldsymbol{W})^{-1}]_{\text{Al. Ge}} \approx 0.25\rho + 0.16\rho^2 + 0.15\rho^3 + 0.13\rho^4 + \dots$$

The coefficients of this expansion has a slower decline for the more fully connected pair (Alabama, Georgia) than for the pair (Alabama, Florida). When 273  $\rho = 0.49$ , this difference is not relevant because the diminishing  $\rho^k$  quickly shrinks the term  $\rho^k[\boldsymbol{W}^k]_{ij}$  towards zero for both pairs. The consequence is 275 that the first few terms, with small k, dominate the series. Considering only 276 the first order approximation with k, we are within 64% and 81% of their limiting values, equal to 0.1915 for the pair (Alabama, Georgia), and equal to 0.1517 for the pair (Alabama, Florida), respectively. Using a third degree 279 approximation with k=3, we get very close to these limits, within 93% and 280 96%, respectively. 281

This picture changes substantially when  $\rho = 0.97$ . Now, even relatively large 282 k-th order neighborhoods contribute a fair amount to the series sum. As a 283 consequence, the convergence of  $[(\boldsymbol{I} - \rho \boldsymbol{W})^{-1}]$  is slow. With k = 1, we are 284 within only 13% and 25% from their limiting values, equal to 1.9030 for the pair (Alabama, Georgia), and equal to 0.9526 for the pair (Alabama, Florida), 286 respectively. Increasing to k = 10 we are still away from the limiting values, 287 58% from (Alabama, Georgia), and 66% from (Alabama, Florida). This means 288 that more geographically distant neighborhood structures, reflected in the ksteps paths from i to j in the  $\mathbf{W}^k$  entries, have a non-negligible impact on 290 the series' limits. Since these paths are different for the two pairs of areas, the 291 end result is that an initial ordering of correlations when  $\rho = 0.49$  is switched 292 as  $\rho$  increases to 0.97.

Let us turn our attention to the relationship between variances  $Var(y_i)$  and the number  $d_i$  of first order neighbors. Wall (2004) noticed that there is a typical negative relationship between these two quantities but that there is also variation of  $Var(y_i)$  among areas with equal  $d_i$ . We use again the approximation in (12) to clarify this in the case of the CAR model.

Suppose that the  $\boldsymbol{W}^k$  converge fast enough such that

$$\operatorname{Var}(y_i) = \frac{\sigma_c^2}{d_i} \left[ (\boldsymbol{I} - \rho \boldsymbol{W})^{-1} \right]_{ii}$$

$$\approx \frac{\sigma_c^2}{d_i} \left( 1 + \rho [\boldsymbol{W}]_{ii} + \rho^2 [\boldsymbol{W}^2]_{ii} + \frac{d_i \rho^3}{D(1 - \rho)} \right)$$

$$= \frac{\sigma_c^2}{d_i} \left( 1 + \rho^2 [\boldsymbol{W}^2]_{ii} \right) + \frac{\sigma_c^2 \rho^3}{D(1 - \rho)}$$

$$\approx \frac{\sigma_c^2}{d_i} \left( 1 + \frac{\rho^2}{d_i} \sum_k \frac{a_{ik} a_{ki}}{d_k} \right)$$

where, in the last approximation, we ignored the last term and used (12).

Therefore, the declining value of  $Var(y_i)$  with  $d_i$  is obvious but we also need

to recognize the effect of the second (and higher) neighborhood order. The

sum  $\sum_k (a_{ik}a_{ki})/d_k$  depends on its number of terms. That is, it depends on the

number  $d_i$  of first order neighbors  $k \sim i$ . It also depends on the connectedness

degree of these neighbors through their  $d_k$  values.

To illustrate with an extreme case, suppose that area i has a single neighbor, area k. Then

Var
$$(y_i) \approx \sigma_c \left( 1 + \frac{\rho^2}{d_k} \right)$$

Two areas in this same single-neighbor situation have different variances if their single neighbors have different number of neighbors. The more connected is the single neighbor k, the smaller the variance of i.

Concerning the negative pairwise correlations, again the spatial dependence parameter  $\rho_c$  and the higher order neighboring areas are crucial to understand 314 their behavior. For  $-1 < \rho_c < 0$ , the terms in the series (10) alternate signs and 315 this explains the counter intuitive behavior of some pairs of areas. If  $\rho$  is close 316 to its lower bound -1, the decay  $\rho^k$  is slow and more distant neighborhood 317 patterns impact on the correlation value with alternating signs. The first term 318  $\rho[\mathbf{W}]_{i,j}$  in the covariance expansion (10) is obviously negative. However, since  $[\boldsymbol{W}^k]_{i,j}$  is not a monotone decreasing function of k, it is possible that the sum of the first two brings the covariance closer to zero or even positive. This 321 happens if an increase in  $[\boldsymbol{W}^2]_{i,j}$  with respect to  $[\boldsymbol{W}]_{i,j}$  more than compensates 322 the decrease from  $|\rho|$  to  $\rho^2$ . This argument is valid with higher order of k.

As an example, consider Vermont and Massachussetts. When  $\rho_c = -0.99999$ , the correlation between these two areas is equal to -0.1051. The convergence of  $[(\boldsymbol{I} - \rho \boldsymbol{W})^{-1}]_{ij}$  for this pair is very slow. Table 2 shows the values  $\boldsymbol{W}^k$ ,  $\rho^k \boldsymbol{W}^k$ , and the cumulative sum  $\sum_{j=0}^k \rho^j \boldsymbol{W}^j$  for Vermont and Massachusetts. We can see that the cumulative sum alternates widely. The difference between k = 100 and k = 101 for the cumulative sum is in the second devimal place, a substantial value for such a large order k.

All pairs of neighboring areas have negative correlation in the CAR model when  $-1 < \rho_c < 0$ . However, in the SAR model with  $\rho_s = -0.99999$ , Vermont and Massachusetts has correlation equal to 0.0293. We discuss the SAR model in more detail in section 4.3 but it is appropriate to advance some its results here. Similarly to the CAR model, using the power expansion of  $[(I - \rho W)^{-1}]$ 

Table 2 Values of the entries of  $\mathbf{W}^k$ ,  $\rho^k \mathbf{W}^k$ , and the cumulative sum  $\sum_{j=0}^k \rho^j \mathbf{W}^j$  for the pair Vermont and Massachusetts. We consider  $\rho = -0.99999$ .

k	1	2	3	4	5	10	100	101
$ ho^k W^k$	-0.3300	0.1778	-0.1948	0.2061	-0.1729	0.1590	0.0315	-0.0313
CumSum	-0.3300	-0.1556	-0.3504	-0.1442	-0.3172	-0.1151	-0.1671	-0.1984

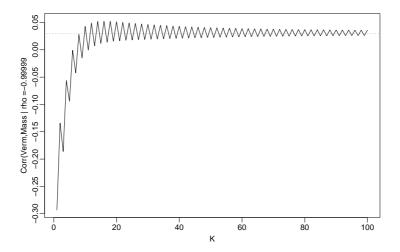


Fig. 2. Successively approximating the correlation between Vermont and Massachusetts as we increase the number of terms in the finite sums of (15), We use  $\rho_s = -0.99999$ .

for the SAR covariance in (5), we can express Cor(i, j) as a power series in  $\rho_s$ .

Figure 2 shows the approximation as successively larger finite sums are used to approximate the eventually positive correlation. Considering only the first

neighborhood orders, the approximation is negative.

The behavior for  $\rho \leq -1$  is less simple to explain with our tools. The series expansion (10) is no longer valid and our interpretations can not be put into use. When an extremely negative spatial parameter is used in the US states graph, the pairwise correlations approach either to -1 or to +1. In Figure 3

we draw the edges according to the limiting behavior of the pairwise corre-344 lation as  $\rho$  approaches its lower bound  $-1.3923 = \min_{i} \{\lambda_i\}^{-1}$ . A virtually 345 identical figure is obtained for the SAR model. Solid lines are used for those pairs in which the correlation approach -1 while the dashed lines represent 347 the pairs with limiting correlation approaching +1. It is not clear what the 348 pattern means but we present a conjecture. It seems as if areas which act 349 as the center of star shaped local neighborhoods have their connecting edges mostly positive. See, for example, Idaho, Colorado, and South Dakota. The 351 edges composing the outer rings of these star-shaped local neighborhoods have 352 negative correlations. 353

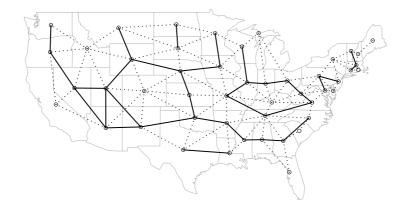


Fig. 3. Edges of US states neighborhod graph drawn according to the pairwise correlation when  $\rho_c$  approaches its lower bound -1.3923. Solid line: positive correlation, +1; dashed line: negative correlation, -1.

To consider an intuitive explanatio for this conjecture, imagine that we are going to assign the value +1 to approximately one half of the areas and -1 to to the remaining areas. In this way we keep the global mean close to zero. Let B the number of neighboring edges connecting areas with different values. If we want to maximize B, it seems that assigning +1 to the center of star shaped areas and -1 to the areas in the outer rings may be near optimal. We

are investigating the truth of our conjecture at the moment.

361 4.3 The SAR model

The arguments for the SAR model are very similar to those presented for the CAR model but the formulas are more convoluted. Using the power series expansion (10) in the SAR covariance (5), we can write

$$\Sigma_{s} = (I - \rho \mathbf{W})^{-1} \Lambda ((I - \rho \mathbf{W})^{-1})'$$

$$= (I + \rho \mathbf{W} + \rho^{2} \mathbf{W}^{2} + \rho^{3} \mathbf{W}^{3} + ...) \Lambda (I + \rho \mathbf{W} + \rho^{2} \mathbf{W}^{2} + \rho^{3} \mathbf{W}^{3} + ...)'$$

$$= \sum_{n=0}^{\infty} \left[ \rho^{n} \sum_{k=0}^{n} \mathbf{W}^{k} \Lambda (\mathbf{W}^{n-k})' \right]$$

365 which has elements given by

$$(\Sigma_s)_{ij} = \frac{\sigma_s}{d_j} \sum_{n=0}^{\infty} \left[ \rho^n \sum_{k=0}^n (\boldsymbol{W}^k)_{ij} (\boldsymbol{W}^{n-k})_{ji} \right] . \tag{15}$$

367 If the third degree approximation for  $(\boldsymbol{I} - \rho \boldsymbol{W})^{-1}$  suffices then

$$(\Sigma_s)_{ij} = \sum_{k=1}^n (I - \rho \mathbf{W} + \rho^2 \mathbf{W} + \rho^3 \mathbf{W}^3)_{ik} \frac{\sigma^2}{d_k} (I - \rho \mathbf{W} + \rho^2 \mathbf{W} + \rho^3 \mathbf{W}^3)_{jk}$$
(16)

where the element  $(\boldsymbol{I} - \rho \boldsymbol{W} + \rho^2 \boldsymbol{W}^2 + \rho^3 \boldsymbol{W}^3)_{ik}$  is equal to

$$(I_{\{i=k\}} - \rho \frac{a_i k}{di} + \frac{\rho^2}{d_i} \sum_{p=1} n \frac{a_{ip} a_{pk}}{d_p} + \frac{\rho^3}{d_i} \sum_{p=1}^n \sum_{q=1}^n \frac{a_{ip} a_{pq} a_{qk}}{d_p d_q})_{ik}$$
(17)

The main difference between SAR and CAR is that a third degree approximation for  $(I - \rho W)^{-1}$  imply in up to a sixth degree polynomial in  $\rho_s$  for each entry of the covariance matrix, the coefficients involving elements of W.

Therefore, we get the same type of polynomial approximation as in the CAR model and our qualitative conclusions follow unchanged for the SAR model.

Incidentally, note that this higher approximating polynomial degree in the SAR model as compared to the CAR model explains why, in Figure 1, the first order neighbor correlatins increase at a slower rate as a function of positive  $\rho_c$  in the CAR model than for positive  $\rho_s$  in the SAR model. For a given approximating polynomial in  $\rho$  for  $(I - \rho W)^{-1}$ , the implied SAR correlation polynomial has more positive terms than the corresponding CAR polynomial, as can be seen in (), for example.

## 383 4.4 The role of $|\lambda_2|$

The second largest eigenvalue modulus  $|\lambda_2|$  is in the interval [0,1) and it is responsible for the speed at which  $[\boldsymbol{W}^k]_{ij}$  converges to its limiting value  $d_j$ . 385 That is, the smaller  $|\lambda_2|$ , the smaller the degree k required in the approxima-386 tion (12). Regular graphs are those with  $d_i$  constant. For a highly irregular 387 neighborhood graph it is difficult to obtain exact results analytically. However, on regular graphs, these results are available and they highlight the interplay 389 between the neighborhood structure and the approximation speed (See Chung, 390 1997, Chapter 1). Basically, the more connected the graph is, the larger the 391 value of  $|\lambda_2|$ . Hence,  $|\lambda_2|$  is a measure of overall connectedness of a graph. In order to illustrate these points, we computed  $|\lambda_2|$  for some regular graphs. 393 Consider a ring graph with nodes  $\{(u, u+1) : 1 \leq u < n^2\} \cup \{(1, n^2)\}.$ 394 Then,  $|\lambda_2| = \cos(2\pi/n^2) \approx 1$  if n is large (Chung, 1997, page 6). This decreases substantially when we pass to a grid graph with  $n^2$  vertices sym-396 metrically wrapped into a torus. In this case, each vertex has four neigh-397 boring vertices and  $|\lambda_2| = (1 + \cos(2\pi/n))/2$ , the midpoint between 1 and 398  $\cos(2\pi/n) < \cos(2\pi/n^2)$  for  $n \geq 2$ . Finally, consider the most dense graph

- possible with  $n^2$  vertices, the complete graph in which every area is a neighbor of every other area. Then,  $|\lambda_2| = 1/(n^2 1) \approx 0$ , if  $n^2$  is large.
- Admittedly, these graphs are highly artificial and do not represent the typical maps found in practice. To have a better idea of the effect of the average density of connections on  $|\lambda_2|$ , and hence on the speed of the convergence  $[\boldsymbol{W}^k]_{ij} \to d_j/D$ , we successively pruned a real map while keeping the entire graph connected. The objective is to show how the value of  $|\lambda_2|$  tends towards 1 as we prune the graph.
- The usual US states map is not the best choice for this demonstration. The 408 reason is that  $|\lambda_2| = 0.9714$  for this graph, a large initial value. This large 409 value indicates that there are parts of the map (such as the NE region) that 410 are hard to reach in a random walk, implying in long paths or a nearly discon-411 nected graph. Even more regularly connected graphs have large eigenvalues. 412 Therefore, in addition to pruning the usual adjacency neighborhood graph, we also added edges between second-order neighbors. That is, we increased the 414 density of connections in the graph by adding edges between areas that are 415 separated from each other by at most a third area. 416
- We randomly selected an edge to be deleted while this was possible until only n-1 edges remained (that is, until we reached a spanning tree). We also randomly created edges between second-order neighbors. To keep the balance on the two directions, we added edges until we reached the same number needed to generate the most pruned graph. We repeated this procedure one hundred times independently.
- Figure 4.4 shows the graph of the second largest eigenvalue modulus  $|\lambda_2(j)|$ where j is either the number of deleted edges from the original map (if j < 0)

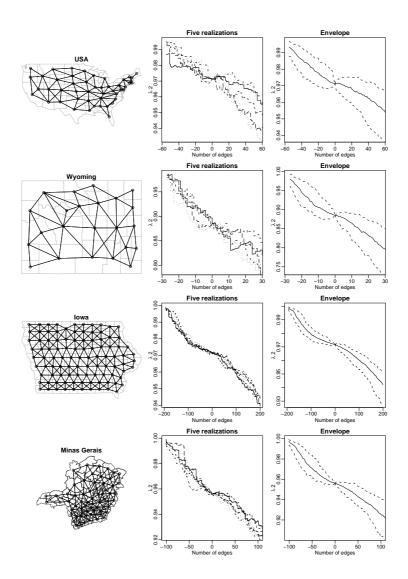


Fig. 4. Successively adding or pruning the adjacency neighborhood graph of four graphs. The geographical regions are the US states map, the the counties of Wyoming and Iowa, and the municipalities of Minas Gerais, a Brazilian state. The second column of plots shows five realizations of the of the addition-pruning process in each graph. The third column of plots shows 95% confidence envelopes based on the simulations in dashed lines, as well as the mean  $|\lambda_2(j)|$  value in solid line.

or the number of added edges (if j>0). We used four geographical regions, shown in the first column of plots: the US states map, the counties of Wyoming and Iowa, and the municipalities of Minas Gerais, a Brazilian state with the same extension as France. Their  $|\lambda_2(0)|$  values are 0.9714, 0.8850, 0.9717, and

0.9561, respectively. The second column of plots shows five realizations of the addition-pruning process in each graph. Each line is the value of  $|\lambda_2(j)|$  as j varies. The third column of plots shows in dashed lines 95% confidence envelopes based on the 100 simulations, as well as the mean  $|\lambda_2(j)|$  value as a solid line.

Specific paths within the confidence envelope are not necessarily monotone.

That is, the deletion (or addition) of a specific edge can decrease (or increase)

the eigenvalue of the resulting *W* matrix. However, the average behavior is

that the denser the connections, the smaller the eigenvalue and hence, faster

the convergence. In terms of the puzzling results discussed in Wall(2004), this

means that the denser the graph, the less likely the change of ranks between

different pairs of areas.

#### 441 5 Conclusions

We found a systematic structure to the SAR and CAR covariance model associated with the spatial structure of the data. This structure is not determined only by the immediate neighborhood of each area. Rather, in a very precise way, we show that the spatial covariance depends on the spatial connections of all neighborhood orders. How strong is the impact of more distant neighboring areas is determined by the second largest eigenvalue modulus of the neighborhood matrix W and the value of the spatial dependence parameter  $\rho$ .

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