## Chapter 7

# Parametric Covariance Structures for Areal Data

This chapter considers parametric covariance structures for areal data. As noted previously, models for the covariance structure of geostatistical data may be adapted for use with areal data simply by replacing (conceptually) each areal site with its centroid or some other representative point. Thus, after making this replacement, the parametric covariance models for geostatistical data developed in the previous chapter may be applied to areal data. But as described in Section 2.3, another, quite different approach to modeling the covariance structure of areal data is through spatial weights matrices. Spatial weights matrices are based upon a specified neighborhood structure for the sites which, when combined with a model such as the SAR, CAR, or SMA model, determine the data's covariance structure. This chapter expands upon Section 2.3 by modeling the elements of the spatial weights matrix (hence also modeling, albeit indirectly, the elements of the covariance matrix) as functions of one or more unknown parameters.

#### 7.1 SAR and CAR models

#### 7.1.1 General requirements of SAR models

Recall from Section 2.3 that the SAR model is given by

$$y_i = \mathbf{x}_i^T \boldsymbol{\beta} + \sum_{j \in \mathcal{N}_i} b_{ij} (y_j - \mathbf{x}_j^T \boldsymbol{\beta}) + d_i, \tag{7.1}$$

or in vector form.

$$y = X\beta + B(y - X\beta) + d,$$

where d is a multivariate normal random vector with mean vector 0 and positive definite diagonal covariance matrix  $\mathbf{K}_{\text{SAR}} = \text{diag}(\kappa_1^2, \dots, \kappa_n^2)$ . The  $b_{ij}$ 's, which are specified (perhaps up to some unknown parameters) by the modeler, relate each observation to the others, with  $b_{ii}$  taken to equal 0 for all i. Equation (7.1) may be rearranged to yield

$$(\mathbf{I} - \mathbf{B})(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = \mathbf{d},$$

and provided that I - B is nonsingular this equation may be manipulated [by premultiplying both sides by  $(I - B)^{-1}$ ] to obtain

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + (\mathbf{I} - \mathbf{B})^{-1}\mathbf{d}.$$
 (7.2)

It follows easily that the covariance matrix of y is

$$\Sigma_{\text{SAR}} = (\mathbf{I} - \mathbf{B})^{-1} \mathbf{K}_{\text{SAR}} (\mathbf{I} - \mathbf{B}^T)^{-1}. \tag{7.3}$$

Clearly this matrix is symmetric; it is also positive definite, for it is the product of a nonsingular matrix, specifically  $(\mathbf{I} - \mathbf{B})^{-1} \mathbf{K}_{\mathrm{SAR}}^{1/2}$  where  $\mathbf{K}_{\mathrm{SAR}}^{1/2} = \mathrm{diag}(\sqrt{\kappa_1^2}, \dots, \sqrt{\kappa_n^2})$ , and its transpose.

The SAR model is sometimes written in a slightly different way, as follows:

$$y = X\beta + u, \quad u = Bu + d \tag{7.4}$$

where **d** is assumed to be distributed as it was in (7.2). From the second equation in (7.4) we obtain  $(\mathbf{I} - \mathbf{B})\mathbf{u} = \mathbf{d}$ , yielding  $\mathbf{u} = (\mathbf{I} - \mathbf{B})^{-1}\mathbf{d}$  (provided that  $\mathbf{I} - \mathbf{B}$  is nonsingular). Substituting this expression for **u** into the first equation in (7.4) yields (7.2), thereby establishing that (7.4) is just another way to write the SAR model.

For future reference, let us summarize the conditions that must be satisfied for  $\Sigma_{SAR}$ , as given by (7.3), to be a valid (symmetric positive definite) SAR covariance matrix. They are:

SAR1:  $K_{SAR}$  is diagonal with positive diagonal elements;

SAR2:  $b_{ii} = 0$  for all i; and margins not aligned

SAR3: I - B is nonsingular.

Note that **B** is not required to be symmetric, which allows the modeler to account for mechanisms thought to operate asymmetrically. For example, if the *i*th response is believed to have twice as much influence on the *j*th response as the *j*th has on the *i*th, then the modeler may take  $b_{ji} = 2b_{ij}$ . Also, **B** and  $\mathbf{K}_{SAR}$  are functionally independent, i.e., how the  $b_{ij}$ 's are specified in no way restricts how the  $\kappa_i^2$ 's must be specified (or vice versa).

#### 7.1.2 General requirements of CAR models

Recall, also from Section 2.3, that the CAR model arises by assuming that for i = 1, ..., n, the conditional distribution of  $y_i$ , given all other responses, is normal with mean

$$E(y_i|y_j, j \neq i) = \mathbf{x}_i^T \boldsymbol{\beta} + \sum_{j \in \mathcal{N}_i} c_{ij} (y_j - \mathbf{x}_j^T \boldsymbol{\beta})$$
 (7.5)

and positive variance  $\kappa_i^2$ , where  $c_{ii}=0$ . Here the  $c_{ij}$ 's play a role analogous to the role that the  $b_{ij}$ 's play in the SAR model, except that they describe spatial dependence for conditional means rather than for the observations themselves. Nevertheless, under certain conditions, the conditional specification yields a model (a joint probability distribution) for the observations. Let  $\mathbf{C}=(c_{ij})$  and  $\mathbf{K}_{\mathrm{CAR}}=\mathrm{diag}(\kappa_1^2,\ldots,\kappa_n^2)$ . Exercise 2.14 established that if  $\mathbf{I}-\mathbf{C}$  is positive definite and  $(\mathbf{I}-\mathbf{C})\mathbf{K}_{\mathrm{CAR}}^{-1}$  is symmetric, then the covariance matrix of  $\mathbf{y}$  is

$$\Sigma_{\text{CAR}} = (\mathbf{I} - \mathbf{C})^{-1} \mathbf{K}_{\text{CAR}},\tag{7.6}$$

and this matrix is positive definite.

A summary of the conditions required for  $\Sigma_{\text{CAR}}$  to be a valid covariance matrix is as follows:

CAR1:  $\mathbf{K}_{CAR}$  is diagonal with positive diagonal elements;

CAR2:  $c_{ii} = 0$  for all i; margins not aligned, for CAR3 and i

CAR3: I - C is positive definite; and

CAR4:  $(I - C)K_{CAR}^{-1}$  is symmetric, or equivalently,  $\frac{c_{ij}}{\kappa_i^2} = \frac{c_{ji}}{\kappa_i^2}$  for all i and j.

Note that conditions CAR1 and CAR2 are identical or completely analogous to SAR1 and SAR2. Condition CAR3, however, is stronger than SAR3, and the symmetry condition CAR4 has no counterpart for SAR models. Furthermore, CAR4 implies that C and K are not functionally independent. Thus, the requirements on C and  $\mathbf{K}_{\text{CAR}}$  to yield a valid covariance matrix in the CAR framework are more stringent than those on B and  $\mathbf{K}_{\text{SAR}}$  in the SAR framework. For example, by CAR1 and CAR4,  $c_{ij}$  and  $c_{ji}$  must have the same sign, whereas there is no such requirement for  $b_{ij}$  and  $b_{ji}$ . Furthermore, CAR4 implies that  $\frac{c_{ij}}{c_{ji}} = \frac{c_{ik}}{c_{ki}} \cdot \frac{c_{kj}}{c_{jk}}$  for all i, j, k for which  $c_{ij} \neq 0$ ,  $c_{ji} \neq 0$ ,  $c_{ik} \neq 0$ ,  $c_{ik} \neq 0$ ,  $c_{jk} \neq 0$ , and  $c_{kj} \neq 0$  (Exercise 7.1). Nevertheless, C is not required to be symmetric.

#### 7.1.3 Relationships to partial correlations

It was noted in Section 2.3 that the off-diagonal elements of the inverse of a covariance matrix  $\Sigma$  are closely related to the partial correlations between two variables, conditioned on the remaining n-2 variables. In fact, it turns out that each off-diagonal element of  $\Sigma^{-1}$ , when divided by the square root of the the product of the two corresponding diagonal elements, is the negative of the aforementioned partial correlation (Whittaker, 1990). That is,

$$\operatorname{corr}(y_i, y_j | y_k, k \neq i, j) = -\frac{\sigma^{ij}}{(\sigma^{ii}\sigma^{jj})^{1/2}}$$
(7.7)

where  $\Sigma^{-1} = (\sigma^{ij})$ . For a CAR model, (7.6) and CAR4 may be used to show that (7.7) reduces to

$$corr(y_i, y_j | y_k, k \neq i, j) = sgn(c_{ij})(c_{ij}c_{ji})^{1/2}$$
(7.8)

(see Exercise 7.2). By (7.8),  $c_{ij}$  and  $c_{ji}$  must satisfy  $0 \le c_{ij}c_{ji} \le 1$  for all i and j. Moreover, (7.8) reveals that by specifying the elements of  $\mathbf{C}$ , the modeler is, in effect, specifying the partial correlations. In particular, specifying that  $c_{ij}$  equals zero specifies that the partial correlation between  $y_i$  and  $y_j$ , conditioned on the remaining observations, is zero. This provides a very useful interpretation of sparse neighbor weighting schemes under a CAR model, namely, that responses taken at sites that are not neighbors are conditionally independent, given the responses at all other sites. Furthermore, (7.8) reveals that if  $c_{ij}$  is taken to be a function of the distance between sites i and j for all i and j, then the partial correlation is also a function of that distance. This implies that it is possible to model the partial correlations as stationary, or even isotropic, using a CAR model.

However, similar statements cannot be made about the zero elements of  $\mathbf{B}$  or stationary modeling of partial correlations via a SAR model because  $\Sigma_{\mathrm{SAR}}^{-1}$  is equal not to  $(\mathbf{I} - \mathbf{B})\mathbf{K}_{\mathrm{SAR}}^{-1}$  but to  $(\mathbf{I} - \mathbf{B})\mathbf{K}_{\mathrm{SAR}}^{-1}(\mathbf{I} - \mathbf{B}^T)$ . Nevertheless, depending on how sparse  $\mathbf{B}$  is, there may still be some pairs of responses that are conditionally independent. Consider, for example, a situation with four observations and a tridiagonal  $\mathbf{B}$ , i.e.,

$$\mathbf{B} = \begin{pmatrix} 0 & b_{12} & 0 & 0 \\ b_{21} & 0 & b_{23} & 0 \\ 0 & b_{32} & 0 & b_{34} \\ 0 & 0 & b_{43} & 0 \end{pmatrix}. \tag{7.9}$$

Then it may be verified (simply by carrying out the multiplication; see Exercise 7.3) that the fourth element in the first row of  $(\mathbf{I} - \mathbf{B})\mathbf{K}_{\mathrm{SAR}}^{-1}(\mathbf{I} - \mathbf{B}^T)$  is equal to zero, implying that the first and fourth observations are conditionally independent, given the second and third observations. However, the first and third observations are not conditionally independent (given the second and fourth observations), in contrast to what would be the case for a CAR with tridiagonal C. For this reason, SAR models are sometimes said to be "less local" than CAR models, meaning that any given response is influenced by more observations under a SAR model, given the same degree of sparsity among the spatial weights.

## 7.2 Parsimonious SAR and CAR models

When fully parameterized, **B** in the SAR model has  $n^2-n$  parameters, and  $K_{SAR}$  has n parameters. Thus, the number of parameters in a SAR model can be as many as  $n^2$ . The number of free parameters in a fully parameterized CAR model is slightly less, due to the restrictions imposed by CAR4, but is still larger than n. It is not possible to sensibly estimate the parameters of such models from the n available observations. Even if many sites have relatively few neighbors, so that many of the elements of **B** or **C** are equal to zero, the data still may be insufficient to support the estimation of their nonzero elements, let alone the diagonal elements of  $K_{SAR}$  or  $K_{CAR}$ . The solution to this problem is to reduce the dimensionality by parameterizing **B**, **C**, and  $K_{SAR}$  or  $K_{CAR}$  using a much smaller set of parameters.

By far the most commonly used and well-studied parameterizations of **B** and **C** are those given by the single multiplicative-parameter forms

$$\mathbf{B} = \rho_{\text{SAR}} \mathbf{W} \quad \text{and} \quad \mathbf{C} = \rho_{\text{CAR}} \mathbf{W},$$
 (7.10)

where  $\mathbf{W} = (w_{ij})$  is a completely specified matrix satisfying  $w_{ii} = 0$  for all i, and  $\rho_{\text{SAR}}$  and  $\rho_{\text{CAR}}$  are unknown real parameters. Despite the use of the same Greek symbol for these parameters as that commonly used to represent a population correlation,  $\rho_{\text{SAR}}$  and  $\rho_{\text{CAR}}$  are not correlations and the temptation to think of them as such must be resisted. We refer to them as the spatial dependence parameters of the SAR and CAR models, though even this term has the potential to mislead if one does not keep in mind that these parameters affect the spatial dependence only indirectly, through the spatial weights matrix.

The parameter spaces for the spatial dependence parameters, i.e., the values of  $\rho_{SAR}$  for which SAR3 holds and the values of  $\rho_{CAR}$  for which CAR3 and CAR4 hold, depend, not surprisingly, on **W**. In particular, they can be expressed in terms of the eigenvalues of **W**. Let  $\{\lambda_i: i=1,\ldots,n\}$  represent those eigenvalues, some of which could be complex. Henceforth assume, as is invariably the case in practice, that at least one site in the spatial dataset has at least one neighbor, so that  $\mathbf{W} \neq \mathbf{0}$ . Then at least one eigenvalue of **W** is nonzero, and, since (by Theorem A.X) the sum of the eigenvalues of **W** is equal to the trace of **W**, actually at least two eigenvalues are nonzero. Furthermore, if **W** is symmetric then all of its eigenvalues are real; if not, then some of its eigenvalues may be complex. In the symmetric case, then, at least one eigenvalue is positive and at least one is negative.

For a SAR model with  $\mathbf{B} = \rho_{\text{SAR}}\mathbf{W}$ , SAR3 specializes to the condition that  $\mathbf{I} - \rho_{\text{SAR}}\mathbf{W}$  is nonsingular. It can be shown (see Exercise 7.4) that this condition is satisfied if and only if  $\rho_{\text{SAR}}$  is not the reciprocal of any real nonzero eigenvalue of  $\mathbf{W}$ . Thus, if A denotes the subset of eigenvalues of  $\mathbf{W}$  that are real and nonzero, then the parameter space for  $\rho_{\text{SAR}}$  is  $\Omega_{\text{SAR}} \equiv \{\rho_{\text{SAR}} : \rho_{\text{SAR}} \neq \lambda_i^{-1}, \lambda_i \in A\}$ . If all the eigenvalues of  $\mathbf{W}$  are complex or zero, there are no constraints on  $\rho_{\text{SAR}}$ .

The parameter space for  $\rho_{\text{CAR}}$  can also be expressed in terms of the eigenvalues of **W**, but due to CAR3 it is more restricted than that for  $\rho_{\text{SAR}}$ , and due to CAR4 it has implications for the main diagonal elements of  $\mathbf{K}_{\text{CAR}}$  (see below). Furthermore, the additional restrictions  $\frac{w_{ij}}{w_{ji}} = \frac{w_{ik}}{w_{ki}} \cdot \frac{w_{kj}}{w_{jk}}$  for all i, j, k for which  $w_{ij} \neq 0$ ,  $w_{ji} \neq 0$ ,  $w_{ik} \neq 0$ ,  $w_{ki} \neq 0$ ,  $w_{jk} \neq 0$ , and  $w_{kj} \neq 0$  must be placed on **W** for CAR4 to hold, although **W** need not be symmetric. Under CAR4, the eigenvalues of **W** are real and may be ordered as follows:

$$\lambda_1 \le \lambda_2 \le \dots \le \lambda_n$$

where  $\lambda_1$  is negative and  $\lambda_n$  is positive (Exercise 7.5a). CAR3 requires that all of the eigenvalues of  $I - \rho_{\text{CAR}}W$  be positive, and Exercise 7.5b establishes that a necessary and sufficient condition for this to happen is  $\lambda_1^{-1} < \rho_{\text{CAR}} < \lambda_n^{-1}$ . Thus, the parameter space for  $\rho_{\text{CAR}}$  is  $\Omega_{\text{CAR}} \equiv \{\rho_{\text{CAR}} : \lambda_1^{-1} < \rho_{\text{CAR}} < \lambda_n^{-1}\}$ . Note that this parameter space includes 0.

The parameter spaces we have specified for  $\rho_{\text{SAR}}$  and  $\rho_{\text{CAR}}$  are the largest allowable, but in practice modelers sometimes use proper subsets of these spaces. For a SAR in particular, if **W** is symmetric the parameter space for  $\rho_{\text{SAR}}$  is often taken to be identical to that for  $\rho_{\text{CAR}}$ , i.e.,  $(\lambda_1^{-1}, \lambda_n^{-1})$ . This choice does exclude many valid SAR models, however.

For parameterizing  $\mathbf{K}_{\mathrm{SAR}}$  there is complete flexibility (subject to SAR1), owing to its functional independence from  $\mathbf{B}$ . One common parsimonious choice is  $\mathbf{K}_{\mathrm{SAR}} = \sigma^2 \mathbf{K}_0$  for some fully specified diagonal matrix  $\mathbf{K}_0$  with positive diagonal elements and some unknown parameter  $\sigma^2 > 0$ . If  $\kappa_i^2$  is believed to be directly (or inversely) proportional to the area  $|S_i|$  of site i for all i, then the modeler might take the diagonal elements of  $\mathbf{K}_0$  to be those areas (or their reciprocals). In human population studies, a similar approach could be taken using not the area but the population size within the site. In the absence of such information, modelers often take  $\mathbf{K}_0 = \mathbf{I}$ . There is less flexibility in parameterizing  $\mathbf{K}_{\mathrm{CAR}}$ . In fact, CAR4 completely determines  $\mathbf{K}_{\mathrm{CAR}}$ , up to a scalar multiple, in terms of the elements of  $\mathbf{C}$ . Specifically, when  $\mathbf{C} = \rho_{\mathrm{CAR}}\mathbf{W}$ , the  $\kappa_i^2$ 's must satisfy  $\kappa_i^2/\kappa_j^2 = w_{ij}/w_{ji}$  for all i and j such that  $w_{ij} \neq 0$ . Thus, if  $\mathbf{W}$  is symmetric, then  $\mathbf{K}_{\mathrm{CAR}}$  must be of the form  $\sigma^2\mathbf{K}^* = \sigma^2\mathrm{diag}(\kappa_1^{*2}, \ldots, \kappa_n^{*2})$  for some  $\sigma^2 > 0$ , where  $\kappa_i^{*2} = 1$  if  $w_{ij} \neq 0$  for at least one j, and  $\kappa_i^{*2}$  is positive but otherwise arbitrary if  $w_{ij} = 0$  for all j. The special case in which  $\mathbf{K}_{\mathrm{CAR}}$  has this form and the  $w_{ij}$ 's are binary spatial adjacency weights has been called the homogeneous  $\mathbf{CAR}$  model by Cressie and Kapat (2008).

The following example gives the marginal variances and correlations corresponding to  $\Sigma_{SAR}$  and  $\Sigma_{CAR}$  for a scenario in which there are seven sites, as depicted below (the number within the site is its index), and the spatial weights matrix has the single multiplicative-parameter form where **W** is simply a binary adjacency matrix:

	1	
2	3	4
5	6	7

The corresponding spatial weights matrix is

$$\mathbf{W} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}, \tag{7.11}$$

which is symmetric. The most extreme eigenvalues of W are approximately  $\pm 2.524$ , so  $I - \rho W$  is positive definite for  $\rho \in (-0.396, 0.396)$ . If we set  $\rho_{SAR} = 0.3$  and  $K_{SAR} = I$ , then the matrix of marginal SAR variances (on the main diagonal) and correlations (on the off-diagonals) is

$$\begin{pmatrix} 1.83 & 0.49 & 0.69 & 0.49 & 0.40 & 0.51 & 0.40 \\ 2.95 & 0.77 & 0.55 & 0.75 & 0.68 & 0.50 \\ 5.57 & 0.77 & 0.66 & 0.81 & 0.66 \\ 2.95 & 0.50 & 0.68 & 0.75 \\ 2.79 & 0.76 & 0.53 \\ 4.43 & 0.76 \\ 2.79 \end{pmatrix}.$$

Its CAR counterpart, likewise setting  $\rho_{\text{CAR}} = 0.3$  and  $\mathbf{K}_{\text{CAR}} = \mathbf{I}$ , is

We see that the variances and correlations under the SAR model are larger than those under the CAR model with the same spatial dependence parameter. Moreover, although the diagonal elements of  $K_{SAR}$  and  $K_{CAR}$  are equal, the marginal variances are heterogeneous; specifically, they are larger at sites that have more neighbors. This feature, called **topologically-induced heterogeneity** by Tiefelsdorf et al. (1999), is often unrealistic in practice. For a SAR model the heterogeneity among variances can be reduced substantially by an appropriate, non-identity choice of  $K_{SAR}$ . But owing to the restrictions imposed on  $K_{CAR}$  by CAR4, this is not an option for a CAR model. Further discussion of this issue is deferred to the next section.

The top four plots in Figure 7.1 display realizations of observations following the single multiplicative-parameter SAR and CAR models described in this section, all with mean zero and  $K_{SAR} = K_{CAR} = I$ . The spatial support for these displays is a 20 × 20 square grid of sites, with neighbors defined as adjacent sites within rows or columns. The top left plot is a collection of 400 independent and identically distributed standard normal random variables, which may be used as a baseline for comparison. The upper right plot corresponds to a SAR model with  $\rho_{SAR} = 0.2$  and shows discernible positive spatial correlation among the observations, but the correlation in the middle left plot, which corresponds to a SAR model with  $\rho_{SAR} = 0.25$ , appears considerably stronger. The spatial correlation in the middle left plot, which corresponds to a CAR model with  $\rho_{CAR} = 0.25$ , appears to be somewhat weaker than that in the SAR model, despite having the same value of the

spatial dependence parameter. The parameter space for  $\rho_{\text{CAR}}$  in this case is (-0.252824, 0.252824), so 0.25 is very close to the upper bound.

Non-multiplicative single-parameter parameterizations of the spatial weights matrix are possible. For a CAR model, Pettitt et al. (2002) took

$$c_{ij} = \frac{\phi \gamma_{ij}}{1 + |\phi| \sum_{k \in \mathcal{N}_i} \gamma_{ik}} \text{for } j \neq i, \quad \kappa_i^2 = \frac{\sigma^2}{1 + |\phi| \sum_{k \in \mathcal{N}_i} \gamma_{ik}},$$
 (7.12)

where  $\gamma_{ij}$  is a fully specified function of the distance between sites i and j (hence  $\gamma_{ij} = \gamma_{ji}$ ) such that  $\gamma_{ii} = 0$  for all i, and  $\gamma_{ij} \geq 0$  for all i and j; for example,  $\gamma_{ij}$  could be a binary adjacency weight, or it could be the reciprocal of the distance between representative points within sites i and j. Here,  $\phi$  is the single unknown parameter in the weights matrix. In contrast to the multiplicative parameterization in (7.10),  $\phi$  is unconstrained. Therefore, determining the eigenvalues of the possibly asymmetric matrix C is unnecessary. It is left as an exercise (Exercise 7.6) to verify that CAR3 and CAR4 are satisfied for this model.

Occasionally, modelers may use additional parameters in the spatial weights matrix to allow for anisotropies or different strengths of dependence for neighbors of different orders. For example, to allow for anisotropy when sites lie on a regular rectangular grid, we could suppose that

$$\Omega = \rho_1 \mathbf{W}_1 + \rho_2 \mathbf{W}_2$$

where  $\mathbf{W}_1$  and  $\mathbf{W}_2$  are binary row-adjacency and column-adjacency matrices, respectively, and  $\rho_1$  and  $\rho_2$  are spatial dependence parameters corresponding to rows and columns. Of course, an alternative way to allow for anisotropy is to suppose that  $\Omega = \rho \mathbf{W}$  where the neighbor weights are equal to 1 within rows and equal to some user-specifed number (different than 1) within columns. An advantage of the first approach, relative to this alternative, is that it allows the data itself to inform the modeler about the degree of anisotropy. A disadvantage is that the parameter space for a model with a multi-parameter weight matrix typically is considerably more difficult to specify than the parameter space for a single-parameter model.

## 7.3 Standardization of spatial weights

For a binary adjacency spatial weights matrix, such as the one used in the seven-site example of the preceding section,  $y_i$  in (7.1) and  $E(y_i|y_j, j \neq i)$  in (7.5) are sums of neighboring random variables. It may seem more natural, however, to model these quantities as averages, rather than sums, of those random variables. This leads to the idea of row standardization. Most (if not all) applications of row standardization have been within the context of the single multiplicative-parameter weights matrices  $\rho_{\text{SAR}}\mathbf{W}$  and  $\rho_{\text{CAR}}\mathbf{W}$  defined in (7.10), with  $\mathbf{W}$  symmetric besides, hence we limit our consideration to that context. Additional assumptions about the weights must be made to accommodate row standardization, which were not made for the general case. For starters, it must be assumed that  $\mathbf{W} = (w_{ij})$  is nonnegative (a nonnegative matrix is a matrix whose elements are all nonnegative, which is not the same as a nonnegative definite matrix.) It must also be assumed that for each i, a j exists such that  $w_{ij} > 0$ , although we relax this assumption in the following section. Then, we are row-standardizing  $\mathbf{W}$  when we divide the elements in the ith row by the corresponding row sum  $w_{i+} = \sum_{j \in \mathcal{N}_i} w_{ij}$ ,  $i = 1, \ldots, n$ . This results in a new, row-standardized spatial weights matrix  $\overline{\mathbf{W}} = (\bar{w}_{ij})$ , where

$$\bar{w}_{ij} = \frac{w_{ij}}{w_{i+}}.$$

Define

$$\mathbf{D} = \operatorname{diag}\left(\frac{1}{w_{1+}}, \frac{1}{w_{2+}}, \dots, \frac{1}{w_{n+}}\right).$$

Then  $\overline{\mathbf{W}}\mathbf{1} = \mathbf{1}$  and  $\overline{\mathbf{W}} = \mathbf{D}\mathbf{W}$ , as is easily verified. Note also that  $\overline{\mathbf{W}}$  generally is asymmetric, even though  $\mathbf{W}$  is symmetric (by assumption).

Exercise 7.7a establishes that if **W** and  $\overline{\mathbf{W}}$  are as described in the previous paragraph, then the eigenvalues  $\lambda_1, \lambda_2, \ldots, \lambda_n$  of  $\overline{\mathbf{W}}$  (which, as it turns out, are real) satisfy  $|\lambda_i| \leq 1$  for all i and  $\lambda_i = 1$  for some i. Thus, the eigenvalues of  $\overline{\mathbf{W}}$  may be ordered to satisfy

$$-1 \le \lambda_1 \le \lambda_2 \le \dots \le \lambda_n = 1.$$

It follows from this result and the results of the previous section that the parameter space for  $\rho_{\text{CAR}}$  in this case is  $(\lambda_1^{-1}, 1)$ , where  $\lambda_1^{-1} \leq -1$ . For the sake of simplicity, and also to avoid some bizarre behavior (see Section 7.5) of the elements of the marginal covariance matrix when  $\rho_{\text{SAR}}$  and  $\rho_{\text{CAR}}$  are less than -1, modelers often take the parameter spaces for  $\rho_{\text{SAR}}$  and  $\rho_{\text{CAR}}$  to be (-1,1) when using a row-standardized spatial weights matrix. As for the  $\kappa_i^2$ 's, for a row-standardized SAR they are unconstrained (apart from SAR1's positivity requirement), but for a row-standardized CAR of the form described in the previous paragraph, they are constrained by CAR4 to have form

$$\kappa_i^2 = \sigma^2 / w_{i+} \tag{7.13}$$

for some  $\sigma^2 > 0$  (Exercise 7.7b). It is customary to take these as the elements of  $K_{SAR}$  for row-standardized SAR models also, though it is not necessary. The special case of a CAR model in which the  $\kappa_i^2$ 's have this form and  $\overline{W}$  is obtained by row-standardizing a binary spatial adjacency weights matrix has been called the weighted CAR model by Cressie and Kapat (2008). The lower left plot in Figure 7.1 displays a realization of such a model, with  $\rho_{CAR} = 0.95$ , on a  $20 \times 20$  square grid. Some spatial correlation is evident in this realization, but there is little that distinguishes the pattern in this plot from that corresponding to a homogeneous CAR model (not shown).

Recall from the previous section that when a binary adjacency spatial weights matrix is used and  $\mathbf{K} = \mathbf{I}$ , the marginal variances of observations under the SAR and CAR models tend to increase as the number of neighbors of the sites at which those observations are taken increases. Now, however, consider what happens to the marginal variances when we row-standardize, using the seven-site example introduced in the previous section. Row standardization of the  $\mathbf{W}$ -matrix given by (7.11) yields a new spatial weights matrix

$$\overline{\mathbf{W}} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & 0 & \frac{1}{4} & 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \end{pmatrix}.$$

It turns out that the most extreme eigenvalues of  $\overline{\mathbf{W}}$  are  $\pm 1.0$ . With this  $\overline{\mathbf{W}}$  as our spatial weights matrix,  $\rho_{\text{SAR}} = 0.8$ , and  $\mathbf{K}_{\text{SAR}}$  given by (7.13), the matrix of marginal variances (on the main

diagonal) and correlations (on the off-diagonals) for the row-standardized SAR model is

Its row-standardized CAR counterpart is

We see, as we also saw when binary adjacency weights without row standardization were used, that the marginal variances and correlations are larger for the SAR model than for the CAR model. More importantly, however, and in contrast to the unstandardized case, row standardization yields marginal variances that are inversely related to the number of neighbors. In general, the marginal variances of row-standardized SAR and CAR models are largest at the margins of the study area and tend to decrease toward its interior. This feature is often as unrealistic as the aforementioned opposite situation that occurs when weights are not row-standardized. In most cases, the modeler would prefer to model the marginal variances as homogeneous, either because of a belief that the data satisfy (approximately) a second-order stationarity assumption, or simply as a result of a lack of prior knowledge that any observations are more (or less) reliable than any others. For this reason, Tiefelsdorf et al. (1999) introduced an alternative standardization scheme that stabilizes (approximately) the variances. The variance-stabilizing spatial weights matrix, denoted by  $\widetilde{\mathbf{W}} = (\widetilde{w}_{ij})$ , is a spatial weights matrix for which

$$\widetilde{w}_{ij} = \frac{w_{ij}}{\left(\sum_{j \in \mathcal{N}_i} w_{ij}^2\right)^{1/2}}.$$
(7.14)

CAR4 requires that the corresponding matrix  $K_{CAR}$  has ith diagonal element

$$\frac{\sigma^2}{\left(\sum_{j\in\mathcal{N}_i}w_{ij}^2\right)^{1/2}}$$

for some  $\sigma^2 > 0$ .

To illustrate, consider yet again the seven-site example, for which the most extreme eigenvalues of  $\widetilde{\mathbf{W}}$  are  $\pm 1.577957$  and the allowable parameter space for  $\rho_{\text{CAR}}$  is therefore (-0.63373, 0.63373). The marginal correlations of SAR and CAR models with  $\rho_{\text{SAR}} = \rho_{\text{CAR}} = 0.5$  are similar to those of their row-standardized counterparts, so we consider those cases, for which the matrices of marginal

variances and correlations are as follows:

$$\begin{pmatrix} 2.33 & 0.58 & 0.77 & 0.58 & 0.50 & 0.59 & 0.50 \\ 2.65 & 0.80 & 0.61 & 0.82 & 0.73 & 0.57 \\ 3.37 & 0.80 & 0.71 & 0.83 & 0.71 \\ 2.65 & 0.57 & 0.73 & 0.82 \\ 2.61 & 0.81 & 0.60 \\ 3.07 & 0.81 \\ 2.61 \end{pmatrix}$$
 
$$\begin{pmatrix} 1.24 & 0.20 & 0.44 & 0.20 & 0.14 & 0.21 & 0.14 \\ 1.04 & 0.46 & 0.22 & 0.46 & 0.33 & 0.19 \\ 0.97 & 0.46 & 0.33 & 0.48 & 0.33 \\ 1.04 & 0.19 & 0.33 & 0.46 \\ 1.04 & 0.46 & 0.22 \\ 0.98 & 0.46 \\ 1.04 \end{pmatrix}$$

We see that these marginal variances, especially those for the CAR model, are somewhat more homogeneous than the marginal variances for models with either no standardization or row standardization. Better variance stabilization seems to occur if the divisor in the weights given by (7.14) is modified from  $\left(\sum_{j\in\mathcal{N}_i}w_{ij}^2\right)^{1/2}$  to  $\left(\sum_{j\in\mathcal{N}_i}w_{ij}^\alpha\right)^{1/\alpha}$ , where  $\alpha$  is slightly less than 2 for SAR models and slightly greater than 2 for CAR models; see Exercise 7.8.

There is another CAR model, which is related to the weighted CAR model and is called the autocorrelated CAR model (Cressie and Kapat, 2008). For this model, C has the single multiplicative-parameter form  $C = \rho_{CAR}W$  where  $w_{ij}$  is equal to  $\sqrt{w_{j+}}/\sqrt{w_{i+}}$  if  $j \in \mathcal{N}_i$  and is equal to 0 otherwise, and  $\kappa_i^2 = \sigma^2/w_{i+}$  (it is assumed, as it was for the weighted CAR model, that  $w_{i+} > 0$  for all i). The most interesting aspect of this model is that the squared partial correlation of each pair of observations, given the rest, is constant across pairs and equal to  $\rho_{CAR}^2$ . As a consequence,  $-1 < \rho_{CAR} < 1$  for this model (Exercise 7.9a). Moreover, the parameter space for  $\rho_{CAR}$  under this model is identical to what it is under the homogeneous CAR model (Exercise 7.9b).

#### 7.4 Islands

"Islands" refer to sites that have no neighbors. If site i is an island, then the ith rows of  $\mathbf B$  and  $\mathbf C$  consist of all zeros, which can cause problems if not dealt with appropriately. For example, the row sum corresponding to an island is zero, which precludes row standardization of the spatial weights matrix for such sites. One possibility for dealing with an island is to simply amalgamate it with the nearest areal unit and combine responses on those units by averaging or summing. But there is some loss of information and potentially some arbitrariness in this approach, as the "nearest" areal unit may not be well defined. Furthermore, combining the islands' responses with those at other sites may result in a probabilistic structure for the observations not consistent with that corresponding to the originally specified neighborhood structure (an exception being when islands are combined only with other islands). Ver Hoef et al. (2018) suggested a more satisfactory approach, which is to take the marginal covariance matrix of the observations to be

$$oldsymbol{\Sigma} = \left( egin{array}{cc} \sigma_I^2 I & 0 \ 0 & \Sigma_M \end{array} 
ight)$$

where the observations are ordered in  $\mathbf{y}$  so that all islands appear first. Here  $\sigma_{\rm I}^2>0$  is the assumed constant variance of responses at islands and  $\Sigma_{\rm M}$  is the SAR or CAR covariance matrix for "mainland" sites, i.e., sites that have neighbors, given by expressions analogous to (7.3) or (7.6). Note that the common variance of responses at islands in this formulation is permitted to be unequal to the variance(s) in  $\Sigma_{\rm M}$ . A slightly more general formulation would allow for heterogeneous variances at islands by assuming that the covariance matrix of responses at islands is  $\sigma^2 \mathbf{K}_{\rm I}$  where  $\mathbf{K}_{\rm I}$  is a specified diagonal matrix with positive diagonal elements. This formulation is consistent with what was described previously in Section 7.2 for the parameterizations of  $\mathbf{K}_{\rm SAR}$  and  $\mathbf{K}_{\rm CAR}$ .

## 7.5 Relationships between spatial weights and marginal correlations

As noted previously, modeling the spatial correlation of areal data using spatial weights matrices is rather more indirect than using a geostatistical model. Although (7.3) and (7.6) express the marginal covariance matrices among the observations for the SAR and CAR models as functions of the spatial weights matrices and **K**, because those expressions involve matrix inverses it is not obvious how the marginal correlations among observations are related to the spatial weights, even when those weights are parameterized parsimoniously. In this section we study this relationship for several scenarios.

Let us consider first the important case where the spatial weights matrix is given by  $\rho \mathbf{W}$ , where **W** is a binary adjacency matrix (hence symmetric),  $\rho$  is either  $\rho_{\text{SAR}}$  or  $\rho_{\text{CAR}}$ , and  $\mathbf{K} = \sigma^2 \mathbf{I}$  for some  $\sigma^2 > 0$ . Figure 7.2 displays the relationship between marginal correlations of neighbors (using the rook's definition) and  $\rho_{SAR}$  or  $\rho_{CAR}$ , for observations on  $\sqrt{n} \times \sqrt{n}$  square lattices, over the interval  $(\lambda_1^{-1}, \lambda_n^{-1})$  for which the CAR covariance matrix is positive definite. (Although SAR models are valid for some  $\rho_{\text{SAR}}$  outside this interval, consideration of the marginal correlations for such models, which behave somewhat erratically, are relegated to Exercise 7.10a.) The upper left panel of the figure indicates that, for the SAR model on a  $3 \times 3$  lattice, the relationship is monotonic, symmetric about 0, nearly linear, and such that the marginal correlation tends to 1 or -1 as  $\rho_{\rm SAR}$  tends to the right or left endpoint of the interval. Only two curves are apparent in this case because there are only two distinct marginal correlations among neighbors for a 3 × 3 lattice: one corresponding to a site-pair in which one site is a corner site, and the other corresponding to a site-pair in which one site is the interior site. The upper right panel of the figure reveals that, for the CAR model on a 3  $\times$  3 lattice, the relationship between the marginal correlations and  $\rho_{\rm CAR}$  is similar to what it is for the SAR model but not quite as linear; in particular, the marginal correlations increase more slowly with  $\rho_{\text{CAR}}$  than with  $\rho_{\text{SAR}}$  over the central portion of the interval, resulting in stronger curvature near the interval's boundaries. Thus, a somewhat larger  $\rho_{\text{CAR}}$  than  $\rho_{\text{SAR}}$  is needed to yield an appreciable marginal correlation. The bottom pair of panels in Figure 7.2 correspond to a  $6 \times 6$  lattice. When compared to the top pair, they suggest that regardless of the size of the lattice, the relationship between the marginal correlations and  $\rho_{SAR}$  (or  $\rho_{CAR}$ ) is qualitatively similar to that seen in the  $3 \times 3$  case, but the curvature near the boundaries of  $(\lambda_1^{-1}, \lambda_n^{-1})$  becomes more pronounced as the size of the lattice increases.

The next figure, Figure 7.3, displays the relationships between the same quantities for scenarios that are exactly the same as those just described except that the original weights have been row-standardized. Accordingly, the parameter space for  $\rho_{\text{CAR}}$  is  $(\lambda_1^{-1}, 1)$ , where it turns out that  $\lambda_1^{-1} = -1$  for both lattices, and the diagonal elements of **K** are given by (7.13). The relationships are qualitatively very similar to what they were when weights were not row-standardized. There is

a feature, however, that is not easily discernible in the figure and was not present previously: some of the curves cross at values of  $\rho$  other than zero. That is, the ranking (from smallest to largest) of the marginal correlations is not consistent over the entire interval. But while this feature is non-intuitive, it is too small to be of much concern to the modeler.

Some additional scenarios with square lattice spatial configurations yield similar results, so they are not displayed here. These scenarios include using anisotropic weights or the queen's definition of neighbors (so that diagonal squares, not merely adjacent squares, are considered neighbors).

Thus, for observations on a square lattice, the dependence of the marginal correlations among neighboring observations on  $\rho_{SAR}$  (or  $\rho_{CAR}$ ), though nonlinear, at least appears to be monotonic over the interval on which  $I - \rho_{CAR}W$  is positive definite. But is the same true for observations on irregular lattices, for which some sites have many more neighbors than others? We answer this question by considering another scenario using the irregular lattice of the 48 contiguous states of the United States of America plus the District of Columbia, which is very similar to a scenario first studied by Wall (2004). Figure 7.4 shows for this lattice the relationship between marginal correlations among neighbors and  $\rho_{SAR}$  (and  $\rho_{CAR}$ ), again over the interval for which the CAR model is positive definite. Spatial weights for the top two panels were binary adjacency weights, for which the relevant interval is (-0.3489, 0.1847); weights for the bottom two panels were rowstandardized, for which the relevant interval is  $(\lambda_1^{-1} = -1.3924, 1)$ . The figure indicates that regardless of whether or not the weights are row-standardized, when  $\rho$  is positive all of the marginal correlations exhibit a nonlinear behavior over the relevant interval similar to that observed for the square lattices, but when  $\rho$  is negative some behave quite differently. In fact, when  $\rho$  is negative, some marginal correlations are positive and decrease as  $\rho$  increases! The state-pairs corresponding to the marginal correlations exhibiting this bizarre behavior are not geographically clustered or otherwise discernibly different, so there is no ready explanation for this phenomenon. In the rowstandardized case, the phenomenon is especially evident over the subinterval (-1.3924, -1). Thus, a modeler could reduce, though not altogether eliminate, such behavior by taking the parameter space for  $\rho$  to be (-1,1) rather than  $(\lambda_1^{-1},1)$ . This is often done in practice.

## 7.6 Variants of SAR and CAR models

The SAR model we have considered so far is but one of several variants and extensions of SAR models that have been proposed in the literature. Furthermore, there is a variant of the CAR model that has received considerable attention. This section briefly describes these variants.

All of the proposed SAR variants are special cases of the **general nested SAR model** given by

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{B}_{\mathrm{Lag}}\mathbf{y} + \mathbf{B}_{\mathrm{Reg}}\mathbf{Z}\boldsymbol{\gamma} + \mathbf{u}, \quad \mathbf{u} = \mathbf{B}_{\mathrm{Err}}\mathbf{u} + \mathbf{d}$$

where  $\mathbf{Z}$ , like  $\mathbf{X}$ , is a specified matrix of regressors;  $\gamma$  is a vector of unknown parameters;  $\mathbf{B}_{\text{Lag}}$ ,  $\mathbf{B}_{\text{Reg}}$ , and  $\mathbf{B}_{\text{Err}}$  are spatial weights matrices that incorporate spatial dependence associated with the response, the regressors, and the errors, respectively; and  $\mathbf{d}$  is a vector whose elements are independent and identically distributed  $\mathbf{N}(0, \sigma^2)$  random variables. A special — but still quite general — case of this model that includes all of the SAR variants proposed to date is obtained by parameterizing each spatial weights matrix using a single parameter, yielding

$$y = X\beta + \rho_{Lag}Wy + \rho_{Reg}WZ\gamma + \rho_{Err}Wu + d$$

Some special cases of this model that have names are as follows:

• SAR error model ( $\rho_{\text{Lag}} = \rho_{\text{Reg}} = 0$ ):

$$y = X\beta + u$$
,  $u = \rho_{Err}Wu + d$ .

This is the classical SAR model featured earlier in this chapter.

• SAR lag model ( $\rho_{\text{Reg}} = \rho_{\text{Err}} = 0$ ):

$$y = X\beta + \rho_{Lag}Wy + d$$

(Lesage and Pace, 2009).

• SAR lagged X model ( $\rho_{\text{Lag}} = \rho_{\text{Err}} = 0, \rho_{\text{Reg}} = 1, \mathbf{Z} = \mathbf{X}$ ):

$$y = X\beta + WX\gamma + d$$

(Vega and Elhorst, 2015).

• Durbin lag model ( $\rho_{\rm Err} = 0, \rho_{\rm Reg} = 1$ ):

$$y = X\beta + \rho_{Lag}Wy + WZ\gamma + d$$

(Lesage and Pace, 2009). The special case that results upon setting  $\mathbf{Z} = \mathbf{X}$  has been called the SAR mixed model (Kissling and Carl, 2008).

• Durbin error model ( $\rho_{\text{Lag}} = 0, \rho_{\text{Reg}} = 1$ ):

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{W}\mathbf{Z}\boldsymbol{\gamma} + \mathbf{u}, \quad \mathbf{u} = \rho_{\mathrm{Err}}\mathbf{W}\mathbf{u} + \mathbf{d}$$

(Lesage and Pace, 2009).

• Double spatial coefficient model ( $\rho_{\text{Reg}} = 0$ ):

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \rho_{\text{Lag}}\mathbf{W}\mathbf{y} + \mathbf{u}, \quad \mathbf{u} = \rho_{\text{Err}}\mathbf{W}\mathbf{u} + \mathbf{d}.$$

Of the SAR variants, the SAR lag model, Durbin lag model, and double spatial coefficient model allow the spatial weights matrix to smooth the covariates in the model matrix in addition to creating autocorrelation among the responses. As a consequence, those three models are not linear models, i.e., the expectations of the responses are not linear functions of the unknown model parameters. Thus, they fall outside the purview of this book. Furthermore, the SAR lag model and SAR mixed model performed poorly in an empirical study, relative to the SAR error model (Kissling and Carl, 2008), which led Ver Hoef et al. (2018) to discourage their use. The SAR lagged X model is merely a Gauss-Markov linear model with model matrix (X, WX), so it regards the observations as independent and can be estimated by ordinary least squares. The Durbin error model is a mixed linear model with the same parameter space for  $\rho_{\rm Err}$  as the SAR error model, but with model matrix (X, WZ) rather than X.

The conditional formulation (7.5) does not allow for the same types of extensions of the CAR model that were just described for the SAR model. Nevertheless, there is one variant of a CAR model, due to Besag and Kooperberg (1995) and called the intrinsic CAR, or ICAR, model, which has been used very often within a Bayesian hierarchical modelling paradigm. In an ICAR model,  $c_{ij} = w_{ij}/w_{i+}$  in (7.5) and  $\kappa_i^2 = \sigma^2/w_{i+}$ . In the case of binary neighbor weights, for example,

$$c_{ij} = rac{1}{|\mathcal{N}_i|} \quad ext{and} \quad \kappa_i^2 = rac{\sigma^2}{|\mathcal{N}_i|}, \quad i = 1, \dots, n.$$

That is, the conditional mean of the *i*th response, given the rest, is the average response of its neighbors, and the *i*th conditional variance is inversely proportional to the number of neighbors of site *i*. Thus, the ICAR model can be viewed as a limiting case, as  $\rho_{\text{CAR}} \to 1$ , of a single multiplicative-parameter CAR model for which the weights have been row-standardized. However, the ICAR model does not specify a proper joint distribution for **y** because  $(\mathbf{I} - \mathbf{1} \cdot \mathbf{W})\mathbf{1} = \mathbf{0}$ , i.e., the precision matrix is singular. Equivalently, the covariance matrix of **y** does not exist. Consequently, the ICAR model has been relegated for use as an improper prior for spatial random effects in a hierarchical Bayesian model. One reason it is very attractive for that purpose is that its only unknown parameter is  $\sigma^2$ . Of course, this also reduces its flexibility.

## 7.7 Spatial moving average models

As introduced in Section 2.3, a spatial moving average (SMA) model for y is given by

$$y_i = \mathbf{x}_i^T \boldsymbol{\beta} + \sum_{j \in \mathcal{N}_i} m_{ij} d_j + d_i,$$

where the spatial weights matrix is denoted by  $\mathbf{M} = (m_{ij})$  and satisfies  $m_{ii} = 0$  for all i, and the  $d_i$ 's are independent and identically distributed normal variables with mean zero and positive variance  $\kappa_i^2$ . In vector form, the model is

$$y = X\beta + (M + I)d,$$

where d is a multivariate normal random vector with mean vector 0 and positive definite diagonal covariance matrix  $\mathbf{K}_{\text{SMA}} = \text{diag}(\kappa_1^2, \dots, \kappa_n^2)$ . The covariance matrix of the observations is

$$\Sigma_{\text{SMA}} = (\mathbf{M} + \mathbf{I})\mathbf{K}_{\text{SMA}}(\mathbf{M}^T + \mathbf{I}), \tag{7.15}$$

which is positive definite if and only if M + I is nonsingular.

As was true for **B** and **C**, **M** generally has too many parameters to be estimated from the available data, so it is usually parameterized much more parsimoniously. The single multiplicative-parameter model,  $\mathbf{M} = \rho_{\text{SMA}} \mathbf{W}$ , is most commonly used. The parameter space for  $\rho_{\text{SMA}}$  is the set of  $\rho_{\text{SMA}}$ -values for which  $\rho_{\text{SMA}} \mathbf{W} + \mathbf{I}$  is nonsingular, which may be obtained in a fashion rather similar to how the parameter spaces for  $\rho_{\text{SAR}}$  and  $\rho_{\text{CAR}}$  were found. The parameter space so obtained is  $\Omega_{\text{SMA}} = \{\rho_{\text{SMA}} : \rho_{\text{SMA}} \neq -\lambda_i^{-1}, \lambda_i \in A\}$  where A was defined in the description of  $\Omega_{\text{SAR}}$ .

To illustrate, the matrix of marginal variances and correlations for the seven-site example introduced in Section 7.2 following a single multiplicative-parameter model with  $\rho_{\text{SMA}} = 0.3$  is

$$\Sigma_{\text{SMA}} = \begin{pmatrix} 1.09 & 0.08 & 0.49 & 0.08 & 0 & 0.08 & 0 \\ & 1.18 & 0.47 & 0.08 & 0.51 & 0.15 & 0 \\ & & 1.36 & 0.47 & 0.14 & 0.46 & 0.14 \\ & & & 1.18 & 0 & 0.15 & 0.51 \\ & & & & & 1.18 & 0.49 & 0.08 \\ & & & & & & 1.27 & 0.49 \\ & & & & & & & 1.18 \end{pmatrix}.$$

Most of the marginal correlations are small, or even zero. The only appreciable correlations are those between adjacent sites.

Figure 7.5 shows the relationship between  $\rho_{\rm SMA}$  and the marginal correlations among neighbors for sites on a 6 × 6 lattice (top two panels) and the contiguous United States plus the District of Columbia (bottom two panels), using binary adjacency weights and their row-standardized counterparts. In contrast to what was seen previously for the SAR and CAR models, the marginal correlations are well-behaved. However, they are rather limited in their extent, as most of their absolute values are less than 0.5 over the entire parameter space. Thus, very strong marginal correlations may not be adequately modeled via a SMA model.

The lower right panel of Figure 7.1 displays a realization of observations on a  $20 \times 20$  square grid following the single-parameter SMA model described in this section, with  $\rho_{\text{SMA}} = 0.25$ . The spatial correlation among the observations induced by the model is discernible, but relatively weak, reinforcing what was seen in Figure 7.5.

SMA models may be combined with SAR models to form so-called SARMA models. For example, a SARMA error model is of the form

$$y_i = \mathbf{x}_i^T \boldsymbol{\beta} + \sum_{j \in \mathcal{N}_i} b_{ij} (y_j - \mathbf{x}_j^T \boldsymbol{\beta}) + \sum_{j \in \mathcal{N}_i} m_{ij} d_j + d_i,$$
 (7.16)

where  $\mathbf{d} = (d_i)$  is distributed as in the SMA model. Provided that  $\mathbf{I} - \mathbf{B}$  is nonsingular, the covariance matrix of the observations under this model is  $(\mathbf{I} - \mathbf{B})^{-1}(\mathbf{M} + \mathbf{I})\mathbf{K}_{\text{SMA}}(\mathbf{M}^T + \mathbf{I})(\mathbf{I} - \mathbf{B}^T)^{-1}$ ; furthermore, this covariance matrix is positive definite if  $\mathbf{I} + \mathbf{M}$  is nonsingular (Exercise 7.11). Parameterizing  $\mathbf{B}$  and  $\mathbf{M}$  as  $\rho_{\text{SAR}}\mathbf{W}$  and  $\rho_{\text{SMA}}\mathbf{W}$ , respectively, yields a parsimonious SARMA error model with covariance matrix

$$\Sigma_{\text{SARMA}} = (\mathbf{I} - \rho_{\text{SAR}}\mathbf{W})^{-1}(\rho_{\text{SMA}}\mathbf{W} + \mathbf{I})\mathbf{K}_{\text{SMA}}(\rho_{\text{SMA}}\mathbf{W}^T + \mathbf{I})(\mathbf{I} - \rho_{\text{SAR}}\mathbf{W}^T)^{-1}.$$
 (7.17)

Although the temporal antecedents of SARMA models — known as ARMA models — are very commonly used for time series data, SARMA models appear to have been used rather sparingly for spatial data.

## 7.8 Relationships between models

Observe that if  $\mathbf{K}_{SAR} = \mathbf{I}$  in (7.3), then  $\mathbf{\Sigma}_{SAR} = (\mathbf{I} - \mathbf{B})^{-1}[(\mathbf{I} - \mathbf{B})^{-1}]^T = [(\mathbf{I} - \mathbf{B}^T)(\mathbf{I} - \mathbf{B})]^{-1} = (\mathbf{I} - \mathbf{B}^T + \mathbf{B}^T \mathbf{B})^{-1}$ . Some authors, upon comparing this last expression to (7.6), have claimed that any SAR model with spatial weights matrix  $\mathbf{B}$  and  $\mathbf{K}_{SAR} = \mathbf{I}$  is a CAR model with (symmetric) spatial weights matrix  $\mathbf{B} + \mathbf{B}^T - \mathbf{B}^T \mathbf{B}$  and  $\mathbf{K}_{CAR} = \mathbf{I}$ . By the same token, upon comparing (7.3) to (7.15), one might claim that a SAR model with spatial weights matrix  $\mathbf{B}$  and  $\mathbf{K}_{SAR} = \mathbf{I}$  is equivalent to a SMA model with  $\mathbf{M} = (\mathbf{I} - \mathbf{B})^{-1} - \mathbf{I}$  and  $\mathbf{K}_{SMA} = \mathbf{I}$ . Both of these claims are false; see Exercise 7.13. However, it is true that every SAR model is a CAR model with some spatial weights matrix, and every CAR model is a SAR model with some spatial weights matrix; see Exercise 7.14a,c. In fact, Ver Hoef et al. (2018) proved the following, even stronger results:

- Any positive definite covariance matrix may be expressed as the SAR covariance matrix  $(\mathbf{I} \mathbf{B})^{-1} \mathbf{K}_{SAR} (\mathbf{I} \mathbf{B}^T)^{-1}$  for an infinite number of pairs of matrices  $\mathbf{B}$  and  $\mathbf{K}_{SAR}$ ;
- Any positive definite covariance matrix may be expressed as the CAR covariance matrix  $(I C)^{-1}K_{CAR}$  for a unique pair of matrices C and  $K_{CAR}$ .

Using similar techniques it can be demonstrated that any positive definite covariance matrix may also be expressed as the SMA covariance matrix  $(M+I)K_{SMA}(M^T+I)$  for an infinite number of pairs of matrices M and  $K_{SMA}$  (see Exercise 7.14b). Thus, any one of the SAR, CAR, and SMA

models can be written as a model of either of the other two types. Moreover, any geostatistical covariance structure given by one of the models described in Chapter 6 can be obtained via an appropriately constructed SAR, CAR, or SMA model.

Typically, modelers take **B**, **C**, and **M** in their SAR, CAR, and SMA models to be sparse matrices, containing mostly zeros. Although any of these models can be expressed as any other, it is not clear whether a sparse-matrix case of such a model can be obtained from a sparse-matrix case of any of the others. However, Ver Hoef et al. (2018) argued that a SAR model with sparse **B** can indeed be obtained from a CAR model with sparse **C**. A case of the opposite was shown previously in Section 7.1.3, and another, due to Besag (1974), is considered in Exercise 7.15.

### 7.9 Exercises

- 1. Show that CAR4 implies that  $\frac{c_{ij}}{c_{ji}} = \frac{c_{ik}}{c_{ki}} \cdot \frac{c_{kj}}{c_{jk}}$  for all i, j, k for which  $c_{ij} \neq 0$ ,  $c_{ji} \neq 0$ ,  $c_{ik} \neq 0$ ,  $c_{ki} \neq 0$ , and  $c_{kj} \neq 0$ . Use this result to give an example of a matrix C that satisfies CAR1-CAR3 but does not satisfy CAR4 for any K.
- 2. Use (7.6), CAR4, and (7.7) to show (7.8).
- 3. Consider a SAR model with **B** given by (7.9) and any  $\mathbf{K}_{SAR}$  satisfying SAR1. Show that the fourth element in the first row of  $\mathbf{\Sigma}_{SAR}^{-1}$  is equal to zero, implying that the first and fourth observations are conditionally independent, given the second and third observations.
- 4. For a SAR model with the single multiplicative-parameter spatial weights matrix  $\rho_{\text{SAR}}\mathbf{W}$ , show that SAR3 is satisfied if and only if  $\rho_{\text{SAR}}$  is not the reciprocal of any real nonzero eigenvalue of  $\mathbf{W}$ . (This is an extension of Proposition 2(i) of Ver Hoef et al. (2018).)
- 5. For a CAR model with single multiplicative-parameter spatial weights matrix  $\rho_{\text{CAR}}\mathbf{W}$ , show that:
  - (a) CAR4 implies that the eigenvalues of **W** are real, and if they are denoted in ordered fashion as  $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ , then  $\lambda_1$  is negative and  $\lambda_n$  is positive;
  - (b) CAR3 is satisfied if and only if  $\lambda_1^{-1} < \rho_{\text{CAR}} < \lambda_n^{-1}$ .
- 6. Show that CAR3 and CAR4 are satisfied for the unconstrained CAR model given by (7.12).
- 7. Let **W** and  $\overline{\mathbf{W}}$  be spatial weights matrices of the single multiplicative-parameter forms described in Section 7.3 (thus **W** is symmetric), and let  $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$  be the ordered eigenvalues of  $\overline{\mathbf{W}}$ .
  - (a) Show that

$$-1 \le \lambda_1 \le \lambda_2 \le \dots \le \lambda_n = 1.$$

- (b) Show that the diagonal elements of the matrix  $\mathbf{K}_{\text{CAR}}$  corresponding to  $\overline{\mathbf{W}}$  are constrained by CAR4 to have form  $\kappa_i^2 = \sigma^2/w_{i+}$   $(i=1,\ldots,n)$  for some  $\sigma^2 > 0$ .
- 8. For the seven-site example considered in this chapter, show that:
  - (a) the marginal variances of the SAR model with  $\rho_{\text{SAR}} = 0.5$  are better stabilized when the divisor of (7.14) is replaced with  $\left(\sum_{j \in \mathcal{N}_i} w_{ij}^{5/3}\right)^{3/5}$ ;

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- (b) the marginal variances of the CAR model with  $\rho_{\text{CAR}} = 0.5$  are better stabilized when the divisor of (7.14) is replaced with  $\left(\sum_{j \in \mathcal{N}_i} w_{ij}^{5/2}\right)^{2/5}$ .
- 9. For the autocorrelated CAR model described in Section 7.3:
  - (a) Show that if  $-1 < \rho_{\text{CAR}} < 1$ . Hint: use (7.8).
  - (b) Show that CAR3 and CAR4 are satisfied if and only if  $\lambda_1^{-1} < \rho_{\text{CAR}} < \lambda_n^{-1}$ .
- 10. Construct figures analogous to Figure 7.1, showing the marginal correlations corresponding to adjacent site-pairs in  $3 \times 3$  and  $6 \times 6$  square lattices, for each of the following, and comment on each figure:
  - (a) SAR models with **W** a binary adjacency matrix and  $-1 \le \rho_{SAR} \le 1$ ;
  - (b) the unconstrained CAR model with elements of C and K given by (7.12), where  $-20 < \phi < 20$  and  $\gamma_{ij}$  is simply the adjacency indicator variable evaluated at sites i and j;
  - (c) the autocorrelated CAR model with **W** a binary adjacency matrix and  $\lambda_1^{-1} < \rho_{\text{CAR}} < \lambda_n^{-1}$ .
- 11. Explain why the SAR lag model, Durbin lag model, and double spatial coefficient model are not linear models.
- 12. Derive the covariance matrix for the SARMA model given by (7.16) assuming that I B is nonsingular, and establish that it is positive definite if, in addition, M + I is nonsingular.
- 13. What model does the SARMA model with covariance matrix (7.17) reduce to when  $\rho_{SAR} = -\rho_{SMA}$ ?
- 14. Explain the fallacy of each of the following claims:
  - (a) Any SAR model with spatial weights matrix **B** and  $\mathbf{K}_{SAR} = \mathbf{I}$  is a CAR model with spatial weights matrix  $\mathbf{B} + \mathbf{B}^T \mathbf{B}^T \mathbf{B}$  and  $\mathbf{K}_{CAR} = \mathbf{I}$ .
  - (b) Any SAR model with spatial weights matrix  ${\bf B}$  and  ${\bf K}_{SAR}={\bf I}$  also a SMA model with spatial weights matrix  ${\bf M}=({\bf I}-{\bf B})^{-1}-{\bf I}$  and  ${\bf K}_{SMA}={\bf I}$ .
- 15. The following lemma is a straightforward consequence of matrix multiplication: Lemma. If **D** is an  $n \times n$  diagonal matrix and **Q** is an  $n \times n$  square matrix with all zeros on the diagonal, then **DQ** and **QD** have all zeros on the diagonal.
  - (a) Use this lemma to show that any positive definite covariance matrix  $\Sigma$  can be expressed as the covariance matrix of a SAR model for a non-unique pair of matrices B and  $K_{SAR}$ .
  - (b) Similarly, show that any positive definite covariance matrix  $\Sigma$  can be expressed as the covariance matrix of a SMA model for a non-unique pair of matrices M and  $K_{SMA}$ .
  - (c) Show that any positive definite covariance matrix  $\Sigma$  can be expressed as the covariance matrix of a CAR model for a unique pair of matrices  $\mathbf{C}$  and  $\mathbf{K}_{CAR}$ .
- 16. Consider observations on a rectangular lattice wrapped on a torus, so that sites in the top row of the lattice are neighbors of sites in the bottom row (and vice versa) and sites in the leftmost column are neighbors with sites in the rightmost column (and vice versa). Suppose

that  $y_{ij}$ , the random variable in the *i*th row and *j*th column of the lattice, follows the SAR model

$$y_{ij} = \beta_1 y_{i-1,j} + \beta_2 y_{i+1,j} + \beta_3 y_{i,j-1} + \beta_4 y_{i,j-1} + \mathbf{d},$$

where  $var(\mathbf{d}) = \sigma^2 \mathbf{I}$  for some  $\sigma^2 > 0$ . Show that the conditional mean of  $y_{ij}$  given the remaining variables is

$$E(y_{ij}|\{y_{kl},(k,l)\neq(i,j)\}) = (1-\beta_1^2+\beta_2^2+\beta_3^2+\beta_4^2)^{-1}\{(\beta_1+\beta_2)(y_{i-1,j}+y_{i+1,j}) + (\beta_3+\beta_4)(y_{i,j-1}+y_{i,j+1}) - (\beta_1\beta_4+\beta_2\beta_3)(y_{i-1,j-1}+y_{i-1,j+1}) - (\beta_1\beta_3+\beta_2\beta_4)(y_{i-1,j+1}+y_{i+1,j-1}) - \beta_1\beta_2(y_{i-2,j}+y_{i+2,j}) - \beta_3\beta_4(y_{i,j-2}+y_{i,j+2})\},$$

and thus that the specified SAR model for which only adjacent sites are neighbors leads to a CAR model with additional sites as neighbors.

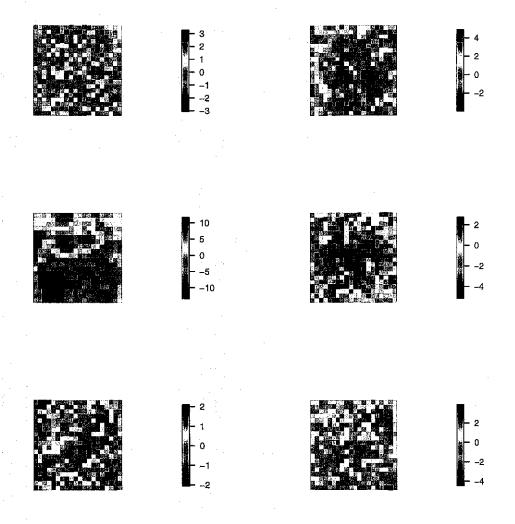


Figure 7.1: Realizations of some SAR, CAR, and SMA processes on a 20 × 20 square grid. Upper left, independent standard normal observations; upper right, SAR model with  $\rho_{\rm SAR}=0.2$ ; middle left, SAR model with  $\rho_{\rm SAR}=0.25$ ; middle right, homogeneous CAR model with  $\rho_{\rm CAR}=0.25$ ; lower left, weighted CAR model with  $\rho_{\rm CAR}=0.95$ ; lower right, SMA model with  $\rho_{\rm SMA}=0.25$ .

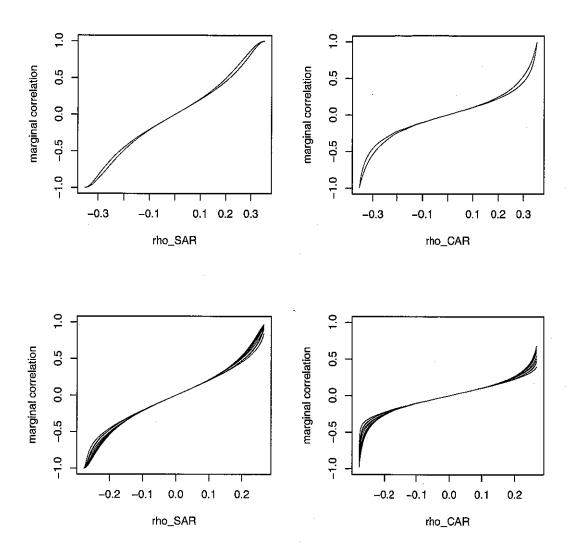


Figure 7.2: Relationship between spatial dependence parameter and marginal correlations of neighbors, under SAR and CAR models, for square lattices with binary spatial weights. Top row:  $3 \times 3$  lattices. Bottom row:  $6 \times 6$  lattices.

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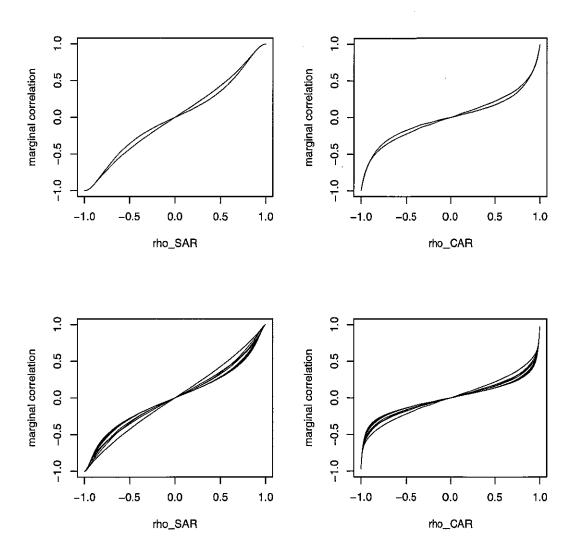


Figure 7.3: Relationship between spatial dependence parameter and marginal correlations of neighbors for square lattices and row-standardized spatial weights. Top row:  $3 \times 3$  lattices. Bottom row:  $6 \times 6$  lattices.

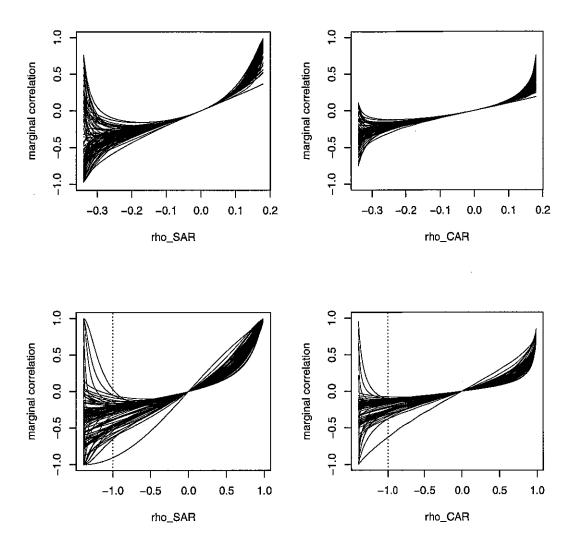


Figure 7.4: Relationship between spatial dependence parameter and marginal correlations of neighbors for states in the contiguous United States of America and the District of Columbia, under SAR and CAR models using binary spatial adjacency weights (top two panels) and row-standardized versions of those spatial weights (bottom two panels). The dotted vertical line in the bottom two plots marks the left endpoint of the parameter space (-1) used in practice by many modelers.

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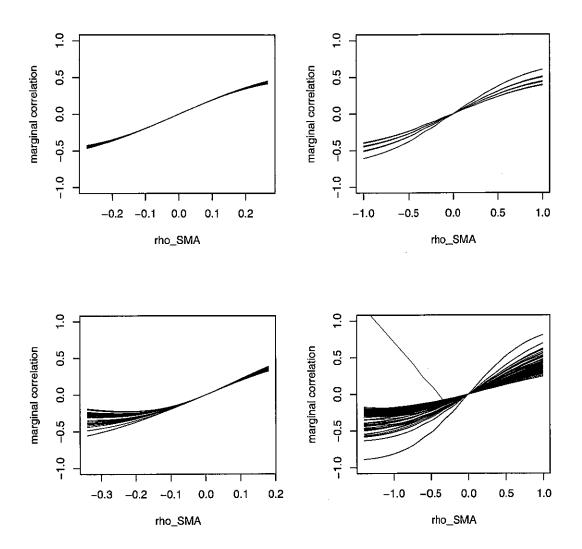


Figure 7.5: Relationship between spatial dependence parameter and marginal correlations of neighbors under SMA models. Top row:  $6 \times 6$  square lattice with binary spatial adjacency weights on the left, and with row-standardized weights on the right. Bottom row: states in the contiguous United States of America and the District of Columbia with binary spatial adjacency weights on the left, and with row-standardized weights on the right.