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On the relationship between conditional (CAR) and simultaneous (SAR) autoregressive models

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ABSTRACT

We clarify relationships between conditional (CAR) and simultaneous (SAR) autoregressive models. We review the literature on this topic and find that it is mostly incomplete. Our main result is that a SAR model can be written as a unique CAR model, and while a CAR model can be written as a SAR model, it is not unique. In fact, we show how any multivariate Gaussian distribution on a finite set of points with a positive-definite covariance matrix can be written as either a CAR or a SAR model. We illustrate how to obtain any number of SAR covariance matrices from a single CAR covariance matrix by using Givens rotation matrices on a simulated example. We also discuss sparseness in the original CAR construction, and for the resulting SAR weights matrix. For a real example, we use crime data in 49 neighborhoods from Columbus, Ohio, and show that a geostatistical model optimizes the likelihood much better than typical first-order CAR models. We then use the implied weights from the geostatistical model to estimate CAR model parameters that provides the best overall optimization.

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1. Introduction

Cressie (1993, p. 8) divides statistical models for data collected at spatial locations into two broad classes: (1) geostatistical models with continuous spatial support, and (2) lattice models, also called

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areal models (Banerjee et al., 2004), where data occur on a (possibly irregular) grid, or lattice, with a countable set of nodes or locations. The two most common lattice models are the conditional autoregressive (CAR) and simultaneous autoregressive (SAR) models, both notable for sparseness of their precision matrices. These autoregressive models are ubiquitous in many fields, including disease mapping (e.g., Clayton and Kaldor, 1987; Cressie and Chan, 1989; Lawson, 2013), agriculture (Cullis and Gleeson, 1991; Besag and Higdon, 1999), econometrics (Anselin, 1988; LeSage and Pace, 2009), ecology (Lichstein et al., 2002; Kissling and Carl, 2008), and image analysis (Besag, 1986; Li, 2009). CAR models form the basis for Gaussian Markov random fields (Rue and Held, 2005) and the popular integrated nested Laplace approximation methods (INLA, Rue et al., 2009), and SAR models are popular in geographic information systems (GIS) with the GeoDa software (Anselin et al., 2006). Hence, both CAR and SAR models serve as the basis for countless scientific conclusions. Because these are the two most common classes of models for lattice data, it is natural to compare and contrast them. There has been sporadic interest in studying the relationships between CAR and SAR models (e.g., Wall, 2004), and how one model might or might not be expressed in terms of the other (Haining, 1990; Cressie, 1993; Martin, 1987; Waller and Gotway, 2004), but there is little clarity in the existing literature on the relationships between these two classes of autoregressive models.

Historically, CAR and SAR models were obtained constructively, which naturally led to results on conditions of the constructions that yielded positive-definite covariance matrices. However, our goal is the opposite. We investigate how to obtain the properties of CAR and SAR models from a positive definite covariance matrix. We aim to clarify, and add to, the existing literature on the relationships between CAR and SAR covariance matrices. Cressie and Wikle (2011, p. 185) show how to obtain a CAR covariance matrix from a geostatistical covariance matrix, and, by extension, from any valid covariance matrix. We add to this by showing that any positive-definite covariance matrix for a multivariate Gaussian distribution on a finite set of points can be written as either a CAR or a SAR covariance matrix, and hence any valid SAR covariance matrix can be expressed as a valid CAR covariance matrix, and vice versa. This result shows that on a finite dimensional space, both SAR and CAR models are completely general models for spatial covariance, able to capture any positive-definite covariance. While CAR and SAR models are among the most commonly-used spatial statistical models, this correspondence between them, and the generality of both models, has not been fully described before now. These results also shed light on some previous literature. CAR and SAR models are often developed with sparseness in mind, where sparseness is the notion that the precision matrix has many zeros, allowing for the use of compact computer storage and fast computing algorithms for sparse matrices. Our results do not necessarily lead to sparse precision matrices for the SAR or CAR specifications, which is a desirable property for these models, so we spend some time investigating this with examples and discussion.

This paper is organized as follows: In Section 2, we review SAR and CAR models and lay out necessary conditions for these models. In Section 3, we provide theorems that show how to obtain SAR and CAR covariance matrices from any positive definite covariance matrix, which also establishes the relationship between CAR and SAR covariance matrices. In Section 4, we provide examples of obtaining SAR covariance matrices from a CAR covariance matrix on fabricated data, and a real example for obtaining a CAR covariance matrix from a geostatistical covariance matrix. Finally, in Section 5, we conclude with a detailed discussion of the incomplete results of previous literature.

2. Review of SAR and CAR models

In what follows, we denote matrices with bold capital letters, and their ith row and jth column with small case letters with subscripts i, j; for example, the i, jth element of $\mathbf{C}$ is $c_{i,j}$. Vectors of fixed values are denoted as lower case bold letters while vectors (or matrices) of random variables are bold, capital, and italic; let $\boldsymbol{Z} \equiv (Z_1, Z_2, \ldots, Z_n)^T$ be a vector of n random variables at the nodes of a graph (or junctions of a lattice). The edges in the graph, or connections in the lattice, define neighbors, which are used to model spatial dependency. Broad reviews of SAR and CAR can be found in Besag (1974), Wall (2004), and Ver Hoef et al. (2018), and in many books (e.g., Anselin, 1988; Haining, 1990; Cressie, 1993; Schabenberger and Gotway, 2005; Cressie and Wikle, 2011; Banerjee et al., 2014).

2.1. SAR models

Consider the SAR model with mean zero. An explicit autocorrelation structure is imposed,

$$\boldsymbol{Z} = \mathbf{B}\boldsymbol{Z} + \boldsymbol{\nu}, \tag{1}$$

where the $n \times n$ spatial weights matrix, $\mathbf{B}$, is relating $\boldsymbol{Z}$ to itself, and $\boldsymbol{\nu} \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Omega})$, where conventionally $\boldsymbol{\Omega}$ is diagonal with positive diagonal values. These models are generally attributed to Whittle (1954). Solving for $\boldsymbol{Z}$, note that conventionally sites do not depend on themselves so $\mathbf{B}$ has zeros on the diagonal, and that $(\mathbf{I} - \mathbf{B})^{-1}$ must exist (Cressie, 1993; Waller and Gotway, 2004), where $\mathbf{I}$ is the identity matrix. Then $\boldsymbol{Z} \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma}_{\mathrm{SAR}})$, where

$$\boldsymbol{\Sigma}_{\mathrm{SAR}} = (\mathbf{I} - \mathbf{B})^{-1}\boldsymbol{\Omega}(\mathbf{I} - \mathbf{B}^T)^{-1}; \tag{2}$$

see, for example, Cressie (1993, p. 409). The spatial dependence in the SAR model is due to the matrix $\mathbf{B}$ which causes the simultaneous autoregression of each random variable on its neighbors. Note that $\mathbf{B}$ does not have to be symmetric because it does not appear directly in the inverse of the covariance matrix (i.e., precision matrix). The covariance matrix must be positive definite. For SAR models, it is enough that $(\mathbf{I} - \mathbf{B})$ is nonsingular (i.e., that $(\mathbf{I} - \mathbf{B})^{-1}$ exists), because the quadratic form, writing it as $(\mathbf{I} - \mathbf{B})^{-1}\boldsymbol{\Omega}[(\mathbf{I} - \mathbf{B})^{-1}]^T$, with $\boldsymbol{\Omega}$ containing positive diagonal values, ensures $\boldsymbol{\Sigma}_{\mathrm{SAR}}$ will be positive definite.

In summary, the following conditions must be met for $\boldsymbol{\Sigma}_{\mathrm{SAR}}$ in (2) to be a valid SAR covariance matrix:

S1 $(\mathbf{I} - \mathbf{B})$ is nonsingular,
S2 $\boldsymbol{\Omega}$ is diagonal with positive diagonal elements, and
S3 $b_{i,i} = 0, \ \forall\, i$.

2.2. CAR models

The term "conditional", in the CAR model, is used because the distribution of each element of the random process is specified conditionally on the values at the neighboring nodes. Let Z_i be a random variable at the ith location, again assuming that the expectation of Z_i is zero for simplicity, and let z_j be its realized value. The CAR model is typically specified as

$$Z_i|\mathbf{z}_{-i} \sim \mathrm{N}\left(\sum_{j=1}^{n} c_{i,j}z_j, m_{i,i}\right), \tag{3}$$

where $\mathbf{z}_{-i}$ is the vector of all z_j where $j \neq i$, $\mathbf{C}$ is the spatial weights matrix with $c_{i,j}$ as its i,jth element, $c_{i,i} = 0$, and $\mathbf{M}$ is a diagonal matrix with positive diagonal elements $m_{i,i}$. Note that $m_{i,i}$ may depend on the values in the ith row of $\mathbf{C}$. In this parameterization, the conditional mean of each Z_i is a weighted linear combination of values at neighboring nodes. The variance component, $m_{i,i}$, often varies with node i, and thus $\mathbf{M}$ is generally heteroscedastic. In contrast to SAR models, it is not obvious that (3) leads to a full joint distribution for $\boldsymbol{Z}$. Besag (1974) used Brook's lemma (Brook, 1964) and the Hammersley–Clifford theorem (Hammersley and Clifford, 1971; Clifford, 1990) to show that, when $(\mathbf{I} - \mathbf{C})^{-1}\mathbf{M}$ is positive definite, $\boldsymbol{Z} \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma}_{\mathrm{CAR}})$, with

$$\boldsymbol{\Sigma}_{\mathrm{CAR}} = (\mathbf{I} - \mathbf{C})^{-1}\mathbf{M}. \tag{4}$$

$\boldsymbol{\Sigma}_{\mathrm{CAR}}$ must be symmetric, requiring

$$\frac{c_{i,j}}{m_{i,i}} = \frac{c_{j,i}}{m_{j,j}}, \quad \forall\, i, j. \tag{5}$$

Most authors describe CAR models as the construction (3), with the condition that $\boldsymbol{\Sigma}_{\mathrm{CAR}}$ must be positive definite given the symmetry condition (5). However, more specific statements are possible

on the necessary conditions for $(\mathbf{I}-\mathbf{C})$, making a comparable condition to S1 for SAR models. We provide a proof, Proposition 1 in the Appendix, showing that if $\mathbf{M}$ is diagonal with positive diagonal elements, along with (5) (forcing symmetry on $\boldsymbol{\Sigma}_{\text{CAR}}$), then $\boldsymbol{\Sigma}_{\text{CAR}}$ is positive definite if and only if $(\mathbf{I}-\mathbf{C})$ has positive eigenvalues. Note that it might be easier to model symmetric $\mathbf{M}^{-1/2}\mathbf{C}\mathbf{M}^{1/2}$, as it establishes a link between $\mathbf{C}$, $\mathbf{M}$, and (5) directly (Cressie and Chan, 1989), and then $(\mathbf{I}-\mathbf{M}^{-1/2}\mathbf{C}\mathbf{M}^{1/2})$ must have positive eigenvalues for $\boldsymbol{\Sigma}_{\text{CAR}}$ to be positive definite (which is used as part of the proof to Proposition 1).

In summary, the following conditions must be met for $\boldsymbol{\Sigma}_{\text{CAR}}$ in (4) to be a valid CAR covariance matrix:

C1 $(\mathbf{I}-\mathbf{C})$ has positive eigenvalues,
C2 $\mathbf{M}$ is diagonal with positive diagonal elements,
C3 $c_{i,i}=0,\ \forall\, i$, and
C4 $c_{i,j}/m_{i,i}=c_{j,i}/m_{j,j},\ \forall\, i,j$.

2.3. Weights matrices

In practice, $\mathbf{B}=\rho_s\mathbf{W}$ and $\mathbf{C}=\rho_c\mathbf{W}$ are usually used to construct valid SAR and CAR models, where $\mathbf{W}$ is a weights matrix with $w_{i,j}\neq 0$ when locations i and j are neighbors, otherwise $w_{i,j}=0$. Neighbors are typically pre-specified by the modeler. When i and j are neighbors, we often set $w_{i,j}=w_{j,i}=1$ (so $\mathbf{W}$ is symmetric), or use row-standardization so that $\sum_{j=1}^{n}w_{i,j}=1$; that is, dividing each row in unstandardized $\mathbf{W}$ by $w_{i,+}\equiv\sum_{j=1}^{n}w_{i,j}$ yields an asymmetric row-standardized matrix that we denote as $\mathbf{W}_+$. For CAR models, define $\mathbf{M}_+$ as the diagonal matrix with $m_{i,i}=1/w_{i,+}$, then (5) is satisfied. The row-standardized CAR model's covariance matrix can be written equivalently as

$$\boldsymbol{\Sigma}_+=\sigma^2(\mathbf{I}-\rho_c\mathbf{W}_+)^{-1}\mathbf{M}_+=\sigma^2(\text{diag}(\mathbf{W1})-\rho_c\mathbf{W})^{-1}, \tag{6}$$

where $\mathbf{1}$ is a vector of all ones, σ^2 is an overall variance parameter, and $\text{diag}(\cdot)$ creates a diagonal matrix from a vector. A special case of the CAR model, called the intrinsic autoregressive model (IAR) (Besag and Kooperberg, 1995), occurs when $\rho_c=1$, but the covariance matrix does not exist, so we do not consider it further.

There can be confusion on how ρ is constrained for SAR and CAR models, which we now clarify. Suppose that $\mathbf{N}$ is a square matrix with real eigenvalues, as would be the case if $\mathbf{N}=\mathbf{W}$ for symmetric $\mathbf{W}$. If $\mathbf{W}$ is asymmetric with possibly complex eigenvalues, then for the CAR covariance matrix (4), Cressie and Chan (1989) use $\mathbf{N}=\mathbf{M}^{-1/2}\mathbf{W}\mathbf{M}^{1/2}$, which is symmetric with real eigenvalues due to CAR condition C4. Note that Li et al. (2012) use $\mathbf{N}=\boldsymbol{\Omega}^{-1/2}\mathbf{W}\boldsymbol{\Omega}^{1/2}$ in the SAR setting (2) and estimate $\boldsymbol{\Omega}$ from data, and deal directly with the possibility of complex eigenvalues. In addition, if $\boldsymbol{\Omega}$ is unconstrained, then condition C4 could be applied for SAR models to $\boldsymbol{\Omega}$ such that $\mathbf{N}=\boldsymbol{\Omega}^{-1/2}\mathbf{W}\boldsymbol{\Omega}^{1/2}$ is symmetric (Wall, 2004). Let $\{\lambda_i\}$ be the set of eigenvalues of $\mathbf{N}$, and let $\{\omega_i\}$ be the set of eigenvalues of $(\mathbf{I}-\rho\mathbf{N})$. Then, in the Appendix (Propositions 2, 3), we show that $\omega_i=(1-\rho\lambda_i)$. Li et al. (2007) note that when all $\lambda_i\neq 0$, $(\mathbf{I}-\rho\mathbf{N})$ will be nonsingular for all $\rho\notin\{\lambda_i^{-1}\}$. However, notice that if $\lambda_i=0$, then $\omega_i=1$ for all ρ. In fact, if all $\lambda_i=0$, then all $\omega_i=1$, and $(\mathbf{I}-\rho\mathbf{N})$ will be nonsingular, satisfying SAR model condition S1. In general, then, $\rho\notin\{\lambda_i{}^{-1}\}$ whenever $\lambda_i\neq 0$ is necessary and sufficient for SAR model condition S1. If any $\lambda_i\neq 0$, then at least two λ_i are nonzero because $\text{tr}(\mathbf{N})=\sum_{i=1}^{n}\lambda_i=0$. If at least two eigenvalues are nonzero, then $\lambda_{[1]}$, the smallest eigenvalue of $\mathbf{N}$, must be less than zero, and $\lambda_{[N]}$, the largest eigenvalue of $\mathbf{N}$, must be greater than zero. Then $1/\lambda_{[1]}<\rho<1/\lambda_{[N]}$ ensures that $(\mathbf{I}-\rho\mathbf{N})$ has positive eigenvalues (Appendix, Propositions 2, 3) and satisfies condition C1 for CAR models.

In practice, the restriction $1/\lambda_{[1]}<\rho<1/\lambda_{[N]}$ is often used for both CAR and SAR models. When considering $\mathbf{W}_+$, the restriction becomes $1/\lambda_{[1]}<\rho<1$ (Haining, 1990, p. 82), where usually $1/\lambda_{[1]}<-1$. Wall (2004) shows irregularities for negative ρ values near the lower bound for both SAR and CAR models, thus many modelers simply use $-1<\rho<1$. In fact, in many cases, only positive autocorrelation is expected, so a further restriction is used where $0<\rho<1$ (e.g., Li et al., 2007). For these constructions, $\boldsymbol{\Sigma}_{\text{SAR}}$ and $\boldsymbol{\Sigma}_{\text{CAR}}$ typically show more positive marginal autocorrelation with

increasing positive ρ values, and more negative marginal autocorrelation with decreasing negative ρ values (Wall, 2004). There has been little research on the behavior of autocorrelation outside of these limits for SAR models.

Weights in $\mathbf{W}$ can be based on distance (Cressie and Chan, 1989) or may be modeled as asymmetric for SAR models (Burden et al., 2015). Cressie et al. (2005) establish a link between $\mathbf{W}$ and $\mathbf{M}$ that allows ρ_c to be constrained and interpreted as a partial correlation parameter when working with spatial rates rather than row-standardization, and this idea, of parameterizing so that ρ_c is a partial correlation, is generalized for numbers of neighbors in the ACAR model of Cressie and Wikle (2011, p. 188). A useful parameterization for CAR models was given by Pettitt et al. (2002); if $\gamma_{i,j}$ represents some function of distance between sites i and j (and often set to zero beyond a certain range), then $\mathbf{C}$ in (4) is constructed as $c_{i,i} = 0$,

$$c_{i,j} = \frac{\phi\gamma_{i,j}}{1 + |\phi| \sum_{j \neq i} \gamma_{i,j}}, \tag{7}$$

for $i \neq j$, and $\mathbf{M}$ in (4) is constructed as

$$m_{i,i} = \frac{1}{1 + |\phi| \sum_{j \neq i} \gamma_{i,j}}. \tag{8}$$

Here, ϕ is an unbounded parameter, obviating the need to find eigenvalues for $\mathbf{C}$.

Our goal is to develop relationships that allow a CAR covariance matrix, satisfying conditions C1–C4, to be obtained from a SAR covariance matrix, satisfying conditions S1–S3, and vice versa. We develop these in the next section, and, in the Discussion and Conclusions section, we contrast our results to the incomplete results of previous literature.

3. Relationships between CAR and SAR models

Assume a covariance matrix for a SAR model as given in (2) and a covariance matrix for a CAR model as given in (4). Cressie and Wikle (2011, p. 185–186) give the result that any Gaussian distribution on a finite set of points, $\boldsymbol{Z} \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma})$, can be written with a covariance matrix parameterized as a CAR model, $\boldsymbol{\Sigma} = (\mathbf{I} - \mathbf{C})^{-1}\mathbf{M}$. We show the additional result that the distribution of $\mathbf{Z}$ can be written as a SAR model with covariance matrix, $\boldsymbol{\Sigma} = (\mathbf{I}-\mathbf{B})^{-1}\boldsymbol{\Omega}(\mathbf{I}-\mathbf{B}^T)^{-1}$. It is straightforward to generalize to the case where the mean is nonzero so, for simplicity of notation, we use the zero mean case. A corollary is that any CAR covariance matrix can be written as a SAR covariance matrix, and vice versa.

We now state the theorems that both SAR and CAR covariance matrices are sufficiently general to represent any finite-dimensional positive-definite covariance matrix. We outline the proofs, which is useful for discussion. Detailed proofs, showing that conditions S1–S3 are satisfied for SAR models, and conditions C1–C4 are satisfied for CAR models, are given in the Appendix.

Theorem 1. *Any positive definite covariance matrix $\boldsymbol{\Sigma}$ can be expressed as the covariance matrix of a SAR model $(\mathbf{I} - \mathbf{B})^{-1}\boldsymbol{\Omega}(\mathbf{I} - \mathbf{B}^T)^{-1}$, (2), for a (non-unique) pair of matrices $\mathbf{B}$ and $\boldsymbol{\Omega}$.*

For a basic outline to the proof of Theorem 1, write $\boldsymbol{\Sigma}^{-1} = \mathbf{L}\mathbf{L}^T$, where $\mathbf{L}$ will be full rank and suppose it has positive diagonal elements. Note that $\mathbf{L}$ is *not* unique. For example, a Cholesky decomposition (Harville, 1997, p. 229) is different from a square-root matrix (Harville, 1997, p. 543), yet either could be used to obtain $\mathbf{L}$, and each will have strictly positive diagonal elements. Decompose $\mathbf{L}$ into $\mathbf{L} = \mathbf{G} - \mathbf{P}$ where $\mathbf{G}$ is diagonal and $\mathbf{P}$ has zeros on the diagonal, so $\mathbf{L}\mathbf{L}^T = (\mathbf{G} - \mathbf{P})(\mathbf{G}^T - \mathbf{P}^T)$. Then set $\boldsymbol{\Omega}^{-1} = \mathbf{G}\mathbf{G}$ and $\mathbf{B}^T = \mathbf{P}\mathbf{G}^{-1}$, so $\boldsymbol{\Sigma}^{-1} = (\mathbf{I} - \mathbf{B}^T)\boldsymbol{\Omega}^{-1}(\mathbf{I} - \mathbf{B})$, expressed in SAR form (2).

The result that follows was given by Cressie and Wikle (2011, p. 185–186), that any multivariate Gaussian distribution can be written as a CAR model. Their construction of the equivalent CAR model corrects an earlier one given by Cressie (1993, p. 434) where the diagonal elements of $\mathbf{C}$ were not necessarily zero.

Theorem 2. *Any positive-definite covariance matrix $\boldsymbol{\Sigma}$ can be expressed as the covariance matrix of a CAR model $(\mathbf{I} - \mathbf{C})^{-1}\mathbf{M}$, (4), for a unique pair of matrices $\mathbf{C}$ and $\mathbf{M}$.*

For a basic outline to the proof of Theorem 2, let $\mathbf{Q} = \boldsymbol{\Sigma}^{-1}$ and decompose it into $\mathbf{Q} = \mathbf{D} - \mathbf{R}$, where $\mathbf{D}$ is diagonal with elements $d_{i,i} = q_{i,i}$ (the diagonal elements of the precision matrix $\mathbf{Q}$), and $\mathbf{R}$ has zeros on the diagonal ($r_{i,i} = 0$) and off-diagonals equal to $r_{i,j} = -q_{i,j}$. Set $\mathbf{C} = \mathbf{D}^{-1}\mathbf{R}$ and $\mathbf{M} = \mathbf{D}^{-1}$. Then $\boldsymbol{\Sigma}^{-1} = \mathbf{D} - \mathbf{R} = \mathbf{D}(\mathbf{I} - \mathbf{D}^{-1}\mathbf{R}) = \mathbf{M}^{-1}(\mathbf{I} - \mathbf{C})$, with $\boldsymbol{\Sigma}$ expressed in CAR form (4).

Having shown that any positive definite matrix $\boldsymbol{\Sigma}$ can be expressed as either the covariance matrix of a CAR model or the covariance matrix of a SAR model, we have the following corollary.

Corollary 1. *Any SAR model can be written as a unique CAR model, and any CAR model can be written as a non-unique SAR model.*

Proof. The proof follows directly by first noting that a SAR model yields a positive-definite covariance matrix, and applying Theorem 2, and then noting that a CAR model yields a positive-definite covariance matrix, and applying Theorem 1. □

The following corollary gives more details on the non-unique nature of the SAR models.

Corollary 2. *Any positive-definite covariance matrix can be expressed as one of an infinite number of* $\mathbf{B}$ *matrices that define the SAR covariance matrix in* (2).

Proof. Write $\boldsymbol{\Sigma}^{-1} = \mathbf{L}\mathbf{L}^T$ as in Theorem 1. Let $\mathbf{A}_{h,s}(\theta)$ be a Givens rotation matrix (Golub and Van Loan, 2013), which is a sparse orthonormal matrix that rotates angle θ through the plane spanned by the h and s axes, where h indexes the row of $\mathbf{A}$, and s indexes the column. The elements of $\mathbf{A}_{h,s}(\theta)$ are as follows. For $i \notin \{h, s\}$, $a_{i,i} = 1$. Also $a_{h,h} = a_{s,s} = \cos(\theta)$, $a_{h,s} = \sin(\theta)$ and $a_{s,h} = -\sin(\theta)$. All other entries of $\mathbf{A}_{h,s}(\theta)$ are equal to zero. That is, $\mathbf{A}_{h,s}(\theta)$ has form

$$\begin{bmatrix}
1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & \cos(\theta) & 0 & \cdots & 0 & \sin(\theta) & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & -\sin(\theta) & 0 & \cdots & 0 & \cos(\theta) & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 1
\end{bmatrix}.$$

Notice that $\boldsymbol{\Sigma}^{-1} = \mathbf{L}\mathbf{L}^T = \mathbf{L}(\mathbf{A}_{h,s}^T(\theta)\mathbf{A}_{h,s}(\theta))\mathbf{L}^T = \mathbf{L}_*\mathbf{L}_*^T$, where $\mathbf{L}_* = \mathbf{L}\mathbf{A}_{h,s}^T(\theta)$. A SAR covariance matrix can be developed as readily for $\mathbf{L}_*$ as for $\mathbf{L}$ in the proof of Theorem 1. Any of the infinite values of $\theta \in [0, 2\pi)$ will result in a unique $\mathbf{A}_{h,s}(\theta)$, leading to a different $\mathbf{L}_*$, and a different $\mathbf{B}$ matrix in (A.1), but yielding the same positive-definite covariance matrix $\boldsymbol{\Sigma}$. □

3.1. Implications of theorems and corollaries

Note that for Corollary 2, additional $\mathbf{B}$ matrices that define a fixed positive-definite covariance matrix in Corollary 2 could also be obtained by repeated Givens rotations. For example, let $\mathbf{L}_* = \mathbf{L}\mathbf{A}_{1,2}^T(\theta)\mathbf{A}_{3,4}^T(\eta)$ for angles θ and η. Then a new $\mathbf{B}$ can be developed for this $\mathbf{L}_*$ just as readily as those in the proof to Corollary 2. We use this idea extensively in the examples.

Theorem 1 helps clarify the use of $\boldsymbol{\Omega}$. Authors often write the SAR model covariance matrix as $(\mathbf{I} - \mathbf{B})^{-1}(\mathbf{I} - \mathbf{B}^T)^{-1}$, assuming that $\boldsymbol{\Omega} = \mathbf{I}$ in (2). In the proofs to Theorem 1 and Corollary 2, this requires finding $\mathbf{L}$ with ones on the diagonal so that $\mathbf{G} = \mathbf{I}$. It is interesting to consider if one can always find such $\mathbf{L}$, which would justify the practice of using the simpler form, $(\mathbf{I} - \mathbf{B})^{-1}(\mathbf{I} - \mathbf{B}^T)^{-1}$, for

SAR models. We now show that this formulation does not allow the use of Theorem 1. Consider the case where the dimensions of the matrices involved are 2×2. Then a matrix $\mathbf{L}$ that has ones on the diagonal, but is otherwise completely general, is

$$\mathbf{L} = \begin{pmatrix} 1 & a \\ b & 1 \end{pmatrix},$$

so

$$\mathbf{L}\mathbf{L}^T = \begin{pmatrix} 1+a^2 & a+b \\ a+b & 1+b^2 \end{pmatrix}.$$

Now the matrix,

$$\begin{pmatrix} 2 & 2 \\ 2 & 5 \end{pmatrix},$$

is positive definite, but is not expressible as $\mathbf{L}\mathbf{L}^T$ if $\mathbf{L}$ is restricted to having ones on the diagonal. We conclude that not every possible positive definite covariance matrix can be written in the form $(\mathbf{I}-\mathbf{B})^{-1}(\mathbf{I}-\mathbf{B}^T)^{-1}$, so $\boldsymbol{\Omega}$ is necessary in $(\mathbf{I}-\mathbf{B})^{-1}\boldsymbol{\Omega}(\mathbf{I}-\mathbf{B}^T)^{-1}$ for Theorem 1 to hold.

In Section 2.3, we discussed how most CAR and SAR models are constructed by constraining ρ in $\rho\mathbf{W}$. Consider Theorem 1, where $\mathbf{L}$ is a lower-triangular Cholesky decomposition. Then $\mathbf{P}$ has zero diagonals and is strictly lower triangular, and so $\mathbf{B}^T = \mathbf{P}\mathbf{G}^{-1}$ is strictly lower triangular. In this construction, all of the eigenvalues of $\mathbf{B}$ are zero. Thus, for SAR models, there are unexplored classes of models that do not depend on the typical construction $\mathbf{B} = \rho\mathbf{W}$.

Most CAR and SAR models are developed such that $\mathbf{C}$ and $\mathbf{B}$ are sparse matrices, containing mostly zeros, but containing positive elements whose weights depend locally on neighbors. Although we demonstrated how to obtain a CAR covariance matrix from a SAR covariance matrix, and vice versa, there is no guarantee that using a sparse $\mathbf{C}$ in a CAR model will yield a sparse $\mathbf{B}$ in a SAR model, or vice versa. Note, however, that Zimmerman and Nunez-Anton (2009, p. 244–245) show how antedependence models, with conditional dependence in one dimension where data are ordered by time, can be viewed as CAR models. These one-dimensional CAR models lead to a sparse Cholesky decomposition (Zimmerman and Nunez-Anton, 2009, Theorem 2.3, p. 41), which would lead to a sparse SAR model formulation. The antedependence models work in more than one dimension, and Zimmerman and Nunez-Anton (2009, Theorem 2.3, p. 41) generalizes to obtaining a sparse Cholesky decomposition from a CAR model. In fact, that is the goal of Rue and Held (2005, Section 2.4, p. 40), who give algorithms to concentrate nonzero values near the diagonal, and show that if an outer (away from the diagonal) triangular part of the matrix $\mathbf{C}$ in a CAR model is all zeros, then that same outer triangular part of $\mathbf{L}$ will also be zeros. We return to this idea in the examples.

4. Examples

We provide two examples, one where we illustrate Theorem 1 primarily, and a second where we use Theorem 2. In the first, we fabricated a simple neighborhood structure and created a positive definite matrix by a CAR construction. Using Givens rotation matrices, we then obtained various non-unique SAR covariance matrices from the CAR covariance matrix. We also explore sparseness in $\mathbf{B}$ for SAR models when they are obtained from sparse $\mathbf{C}$ for CAR models.

For a second example, we used real data on neighborhood crimes in Columbus, Ohio. We model the data with the two most common CAR models, using a first-order neighborhood model where $\mathbf{C}$ is both unstandardized and row-standardized. Then, from a positive-definite covariance matrix obtained from a geostatistical model, we obtain the equivalent and unique CAR covariance matrix. We use the weights obtained from the geostatistical covariance matrix to allow further CAR modeling, finding a better likelihood optimization than both the unstandardized and row-standardized first-order CAR models.

4.1. Uniqueness and sparseness for SAR models

Consider the graph in Fig. 1a, which shows an example of neighbors for a CAR model. Using one to indicate a neighbor, and zeros elsewhere, the $\mathbf{W}$ matrix was used to create the row-standardized $\mathbf{W}_+$ matrix in (6). Values of $\rho_c\mathbf{W}_+$, where $\rho_c = 0.9$, are shown graphically in Fig. 1b. For the resulting covariance matrix, $\boldsymbol{\Sigma}_+$ in (6), the Cholesky decomposition was used to create $\mathbf{L}$ as in Theorem 1. Using (A.1) in Theorem 1, the weights matrix $\mathbf{B}$ created from $\mathbf{L}$ is shown in Fig. 1c. Note from Fig. 1b that, beyond indices separated by more than 5, all elements are zero. Those indices separated by 5 can be seen with a vertical orientation in Fig. 1a. Consequently, the off-diagonal elements in the Cholesky decomposition shown in Fig. 1c, with indices separated by more than 5, are all zero (in keeping with Theorem 2.3, Zimmerman and Nunez-Anton, 2009, p. 41), and many of those indices separated by less than 5 are non-zero "fill-in" values (Rue and Held, 2005, p. 44). One approach to obtain sparseness works by concentrating non-zero values in $\mathbf{W}$ to be near the diagonal by re-indexing the data (Rue and Held, 2005, p. 47). Other approaches include tapering (Furrer et al., 2006) and thresholding (Bickel and Levina, 2008) for covariance matrices (for a broad treatment, see Pourahmadi, 2013).

For the same covariance matrix $\boldsymbol{\Sigma}_+$, we also used the spectral decomposition to create $\mathbf{L}$ as in Theorem 1. The weights matrix $\mathbf{B}$ created from this $\mathbf{L}$, using (A.1) in Theorem 1, is shown in Fig. 1d. Note that the $\mathbf{B}$ matrix in Fig. 1d is less sparse than $\mathbf{B}$ in Fig. 1c, although they both yield exactly the same covariance matrix by the SAR construction (2), which we verified numerically. Fig. 1c, because it is strictly upper triangular, also verifies our comments in Section 3.1; that there exists some $\mathbf{B}$ whose eigenvalues are all zero.

In addition to re-indexing data with the Cholesky decomposition to obtain sparseness, we sought to transform the $\mathbf{B}$ matrix in Fig. 1d to a sparser form using the proof to Corollary 2 and the Givens rotations. For a nonzero vector $\mathbf{x} = (x_1, \ldots, x_n)$, an index of sparseness (Hoyer, 2004) is

$$\text{sparseness}(\mathbf{x}) = \frac{\sqrt{n} - \frac{\sum_i |x_i|}{\sqrt{\sum_i x_i^2}}}{\sqrt{n} - 1},$$

which ranges from zero to one. Ignoring the dimensions of a matrix, we create the matrix function

$$f(\mathbf{B}) = \frac{\sum_{i,j} |b_{i,j}|}{\sqrt{\sum_{i,j} b_{i,j}^2}},$$

which is a measure of the fullness of a matrix. We propose an iterative algorithm to minimize $f(\mathbf{B})$ for orthonormal Givens rotations as explained in Corollary 2. Let $\mathbf{L}_{h,s}(\theta) = \mathbf{L}\mathbf{A}_{h,s}^T(\theta)$, where $\mathbf{L} = \mathbf{V}\mathbf{E}^{-1/2}\mathbf{V}^{-1}$ used the spectral decomposition of $\boldsymbol{\Sigma}_+$ as in the proof of Theorem 1, and $\mathbf{A}_{h,s}(\theta)$ is a Givens rotation matrix as in the proof of Corollary 2. Denote θ_k^* as the value of θ that minimizes $f(\mathbf{B})$ when $\mathbf{B}$ is created by decomposing $\mathbf{L}\mathbf{A}_{h,s}^T(\theta)$ into $\mathbf{P}$ and $\mathbf{G}$ (as in (ii) in Theorem 1), while constraining θ to values satisfying $b_{i,j} \geq 0\ \forall\, i, j$. Then $\mathbf{L}_{1,2}^{[1]} \equiv \mathbf{L}\mathbf{A}_{1,2}^T(\theta_1^*)$, where $k = 1$ is the first iteration. For the second iteration, let θ_2^* be the value that minimizes $f(\mathbf{B})$ for $\mathbf{B}$ created from $\mathbf{L}_{1,2}^{[1]}\mathbf{A}_{1,3}^T(\theta)$, and hence for $k = 2$, $\mathbf{L}_{1,3}^{[2]} \equiv \mathbf{L}_{1,2}^{[1]}\mathbf{A}_{1,3}^T(\theta_2^*)$ where superscript $[k]$ indicates iteration. We cycled through $h = 1, 2, \ldots, 24$ and $s = (h+1), \ldots, 25$ for each iteration k in a coordinate descent minimization of $f(\mathbf{B})$. We cycled through all of h and s eight times for a total of $8(25)(25-1)/2 = 2400$ iterations. The value of $f(\mathbf{B})$ for each iteration is plotted in Fig. 1e and the final $\mathbf{B}$ matrix is given in Fig. 1f. Although we did not achieve the sparsity of Fig. 1c, we were able to increase sparseness from the starting matrix in Fig. 1d. Note that the $\mathbf{B}$ matrix depicted in Fig. 1f yields exactly the same covariance matrix as the $\mathbf{B}$ matrices shown in Fig. 1c, d. There are undoubtedly better ways to minimize $f(\mathbf{B})$, such as simulated annealing (Kirkpatrick et al., 1983), and there may be alternative optimization criteria. We do not pursue these here. Our goal was to show that it is possible to explore many configurations of matrix weights in SAR models, which produce equivalent covariance matrices, by using orthonormal Givens rotations of the $\mathbf{L}$ matrix.

4.2. Columbus crime data

The Columbus data are found in the `spdep` package (Bivand et al., 2013; Bivand and Piras, 2015) for R (R Core Team, 2016). Fig. 2 shows 49 neighborhoods in Columbus, Ohio. We used residential

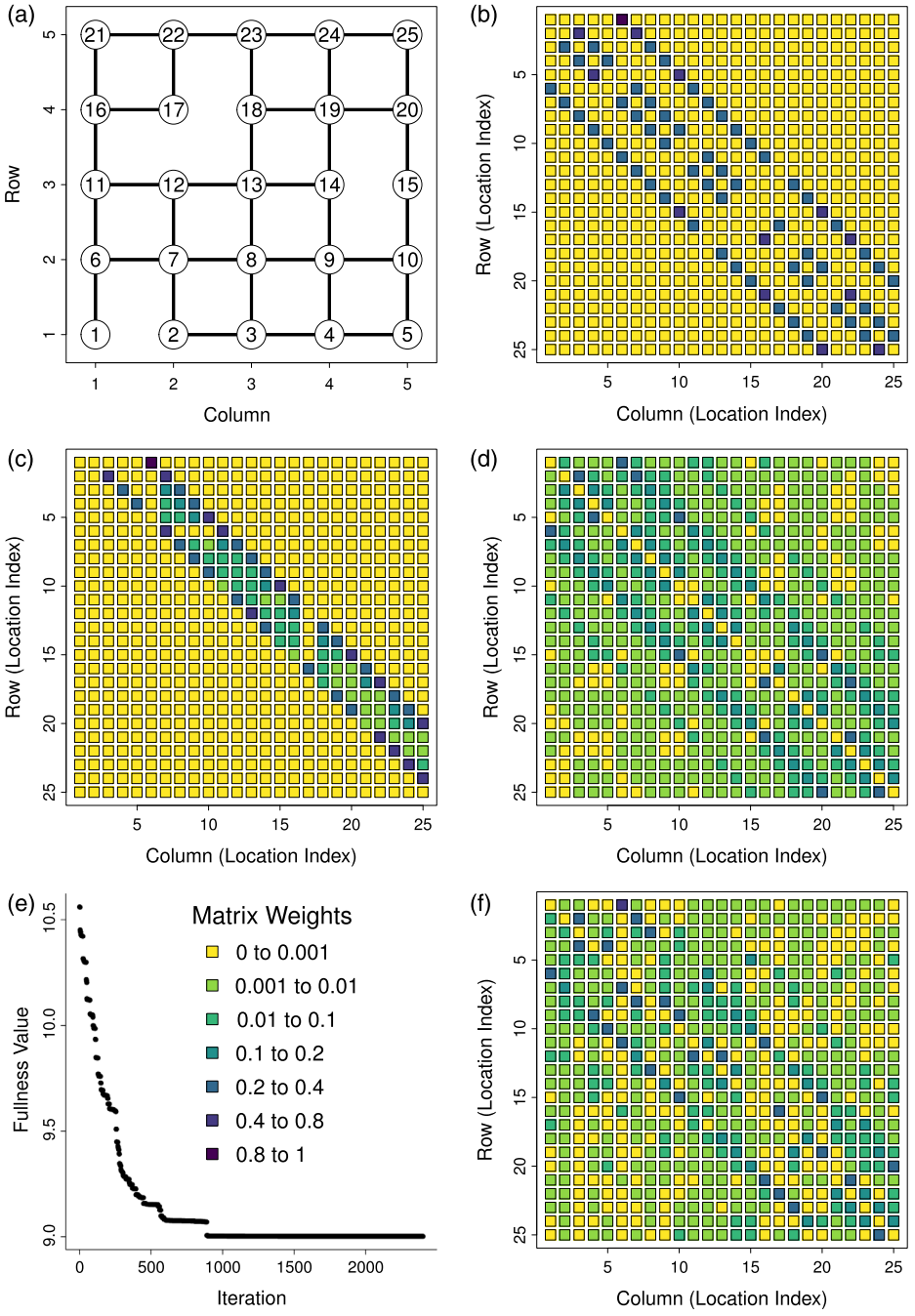

Fig. 1. Sparseness in CAR and SAR models. (a) 5×5 grid of spatial locations, with lines connecting neighboring sites. The numbers in the circles are indices of the locations. (b) Graphical representation of weights in the $\rho\mathbf{W}_+$ matrix in the CAR model. The color legend is given below. (c) Graphical representation of weights in the $\mathbf{B}$ matrix when using the Cholesky decomposition, and (d) when using spectral decomposition. (e) Fullness function during minimization when searching for sparseness. (f) Graphical representation of weights in the $\mathbf{B}$ matrix at the termination of an algorithm to search for sparseness using Givens rotations on the spectral decomposition in (d).

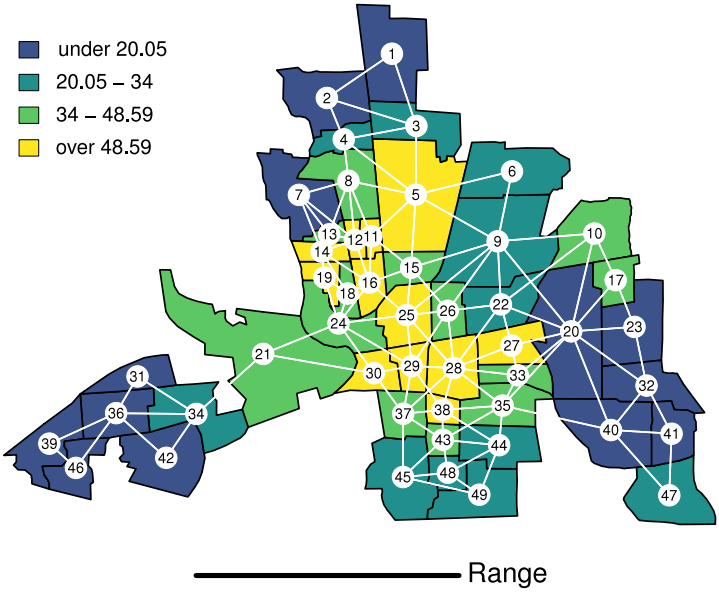

Fig. 2. Columbus crime map, in rates per 1000 people. Numbers in each polygon are the indices for locations, and the white lines show first-order neighbors. The estimated range parameter from the spherical geostatistical model is shown at the bottom.

burglaries and vehicle thefts per thousand households in the neighborhood (Anselin, 1988, Table 12.1, p. 189) as the response variable. Spatial pattern among neighborhoods appeared autocorrelated (Fig. 2), with higher crime rates in the more central neighborhoods. When analyzing rate data, it is customary to account for population size (e.g., Clayton and Kaldor, 1987), which affects the variance of the rates. However, for illustrative purposes, we used raw rates. A histogram of the data appeared approximately bell-shaped, thus we assumed a Gaussian distribution with a covariance matrix containing autocorrelation among locations.

First-order neighbors were also taken from the spdep package for R, and are shown by white lines in Fig. 2. Using a one to indicate a neighbor, and zero otherwise, we denote the 49×49 matrix of weights as $\mathbf{W}_{\text{un}}$, and the CAR precision matrix has $\mathbf{C} = \rho_{\text{un}}\mathbf{W}_{\text{un}}$ and $\mathbf{M} = \sigma^2_{\text{un}}\mathbf{I}$ in (4). Using the eigenvalues of $\mathbf{W}_{\text{un}}$, the bounds for ρ_{un} were $-0.335 < \rho_{\text{un}} < 0.167$. We added a constant independent diagonal component, $\delta^2_{\text{un}}\mathbf{I}$ (also called the nugget effect in geostatistics), so the covariance matrix was $\boldsymbol{\Sigma}_{\text{un}} = \sigma^2_{\text{un}}(\mathbf{I} - \rho_{\text{un}}\mathbf{W}_{\text{un}})^{-1} + \delta^2_{\text{un}}\mathbf{I}$. Denote the crime rates as $\mathbf{y}$. We assumed a constant mean, so $\mathbf{y} \sim \text{N}(\mathbf{1}\mu, \boldsymbol{\Sigma}_{\text{un}})$, where $\mathbf{1}$ is a vector of all ones. Let $\mathcal{L}(\boldsymbol{\theta}_{\text{un}}|\mathbf{y})$ be minus 2 times the restricted maximum likelihood function (REML, Patterson and Thompson, 1971, 1974) for the crime data, where the set of covariance parameters is $\boldsymbol{\theta}_{\text{un}} = (\sigma^2_{\text{un}}, \rho_{\text{un}}, \delta^2_{\text{un}})^T$. We optimized the REML likelihood and obtained $\mathcal{L}(\hat{\boldsymbol{\theta}}_{\text{un}}|\mathbf{y}) = 388.83$. Recall that CAR models are generally heteroscedastic (e.g., Wall, 2004). The marginal variances of the estimated model are shown in Fig. 3a, and the marginal correlations are shown in Fig. 4a.

We also optimized the likelihood using the row-standardized weights matrix, $\mathbf{W}_+$ in (6), which we denote $\mathbf{W}_{\text{rs}}$. In this case, the CAR precision matrix has $\mathbf{C} = \rho_{\text{rs}}\mathbf{W}_+$, $-1 < \rho_{\text{rs}} < 1$, and $\mathbf{M} = \sigma^2_{\text{rs}}\mathbf{M}_+$ in (4). Again we added a nugget effect, so $\boldsymbol{\Sigma}_{\text{rs}} = \sigma^2_{\text{rs}}(\mathbf{I} - \rho_{\text{rs}}\mathbf{W}_+)^{-1}\mathbf{M}_+ + \delta^2_{\text{rs}}\mathbf{I}$. For the set of covariance parameters $\boldsymbol{\theta}_{\text{rs}} = (\sigma^2_{\text{rs}}, \rho_{\text{rs}}, \delta^2_{\text{rs}})^T$, we obtained $\mathcal{L}(\hat{\boldsymbol{\theta}}_{\text{rs}}|\mathbf{y}) = 397.25$. This shows that the unstandardized weights matrix $\mathbf{W}_{\text{un}}$ provides a substantially larger REML likelihood optimization than $\mathbf{W}_{\text{rs}}$. The marginal variances of the row-standardized model are shown in Fig. 3b, and the marginal correlations are shown in Fig. 4b. The difference between $\mathcal{L}(\hat{\boldsymbol{\theta}}_{\text{un}}|\mathbf{y})$ and $\mathcal{L}(\hat{\boldsymbol{\theta}}_{\text{rs}}|\mathbf{y})$ indicates that the weights matrix $\mathbf{C}$ has a substantial effect for these data.

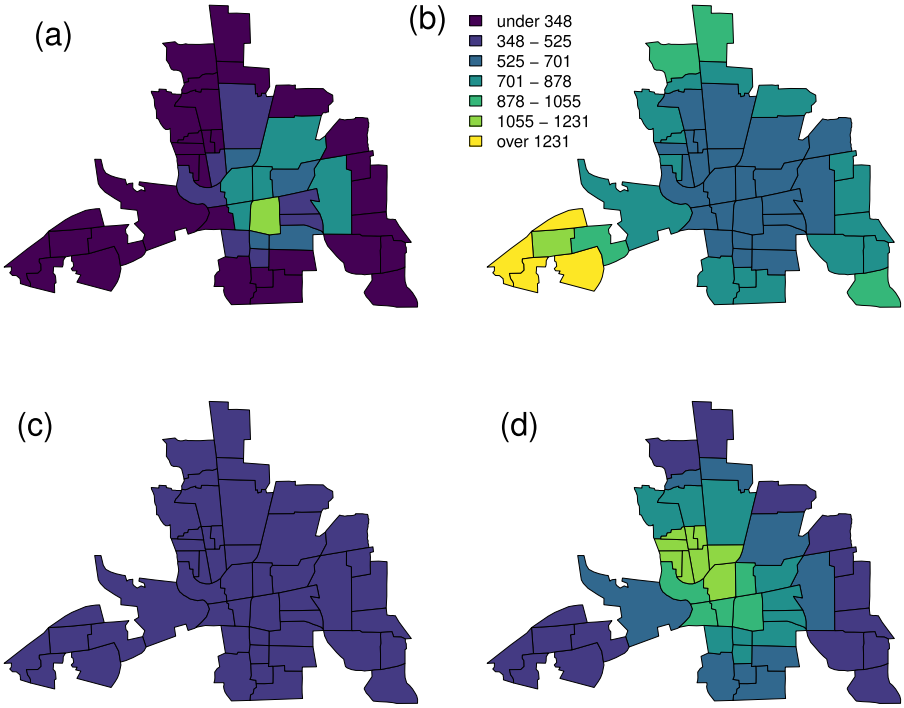

Fig. 3. Marginal variances by location for Columbus crime data. (a) Unstandardized first-order CAR model, (b) Row-standardized first-order CAR model, (c) spherical geostatistical model, (d) CAR model using weights obtained from geostatistical model.

To show that a CAR covariance matrix can be developed from any covariance matrix (Theorem 2), next we fit a geostatistical model and derive the corresponding CAR covariance matrix. We optimized the likelihood with a geostatistical model using a spherical autocorrelation model. Denote the geostatistical correlation matrix as $\mathbf{S}$, where

$$s_{i,j} = [1 - 1.5(e_{i,j}/\alpha) + 0.5(e_{i,j}/\alpha)^3]\mathcal{I}(d_{i,j} < \alpha),$$

and $\mathcal{I}(\cdot)$ is the indicator function, equal to one if its argument is true, otherwise it is zero, and $e_{i,j}$ is Euclidean distance between the centroids of the ith and jth polygons in Fig. 2. We included a nugget effect, so $\boldsymbol{\Sigma}_{\text{sp}} = \sigma^2_{\text{sp}}\mathbf{S} + \delta^2_{\text{sp}}\mathbf{I}$. For the set of covariance parameters $\boldsymbol{\theta}_{\text{sp}} = (\sigma^2_{\text{sp}}, \alpha, \delta^2_{\text{sp}})^T$, we obtained $\mathcal{L}(\hat{\boldsymbol{\theta}}_{\text{sp}}|\mathbf{y}) = 374.61$. The geostatistical model provides a substantially better optimized likelihood than either the unstandardized or row-standardized CAR model. The marginal variances of geostatistical models are equal (Fig. 3c). The estimated range parameter, $\hat{\alpha}$, is shown by the lower bar in Fig. 2. Responses at locations separated by a distance greater than that shown by the bar are estimated to have zero correlation (Fig. 4c).

It appears that the geostatistical model provides a much better optimized likelihood than the two most commonly-used CAR models. Others have compared CAR to geostatistical models (e.g., Banerjee et al., 2003; Hrafnkelsson and Cressie, 2003; Song et al., 2008), and Rue and Tjelmeland (2002) and Cressie and Verzelen (2008) use a "closeness" criteria to approximate a geostatistical model with a CAR model, but where they enforce some sparsity in the CAR weight matrix. Here, we try another way to find a CAR model to compete with the geostatistical model, but where the weight matrix is not sparse. Using Theorem 2, as in Cressie and Wikle (2011, p. 185), we created $\mathbf{C}_{\text{cg}}$ and $\mathbf{M}_{\text{cg}}$ as in (A.2) in the Appendix from the positive definite covariance matrix of the geostatistical model, $\boldsymbol{\Sigma}_{\text{sp}} = (\mathbf{I} - \mathbf{C}_{\text{cg}})^{-1}\mathbf{M}_{\text{cg}}$. Here, we have a CAR representation that is equivalent to the spherical

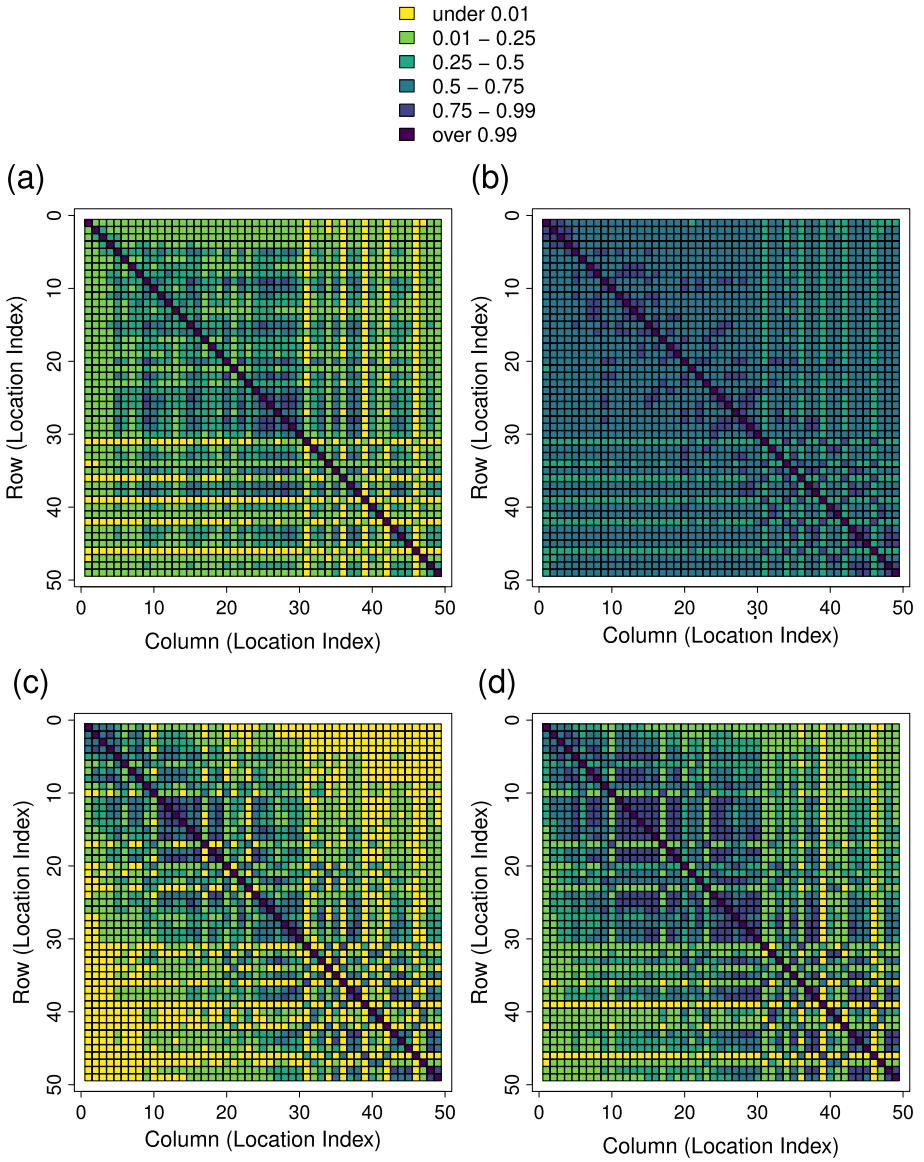

Fig. 4. Marginal correlations for Columbus crime data, none of which were below zero. The location indices are given by the numbers in Fig. 2. (a) Unstandardized first-order CAR model, (b) Row-standardized first-order CAR model, (c) spherical geostatistical model, (d) CAR model using weights obtained from geostatistical model.

geostatistical model. Now consider scaling $\mathbf{C}_{cg}$ with ρ_{cg}, so $\boldsymbol{\Sigma}_{cg} = \sigma^2_{cg}(\mathbf{I} - \rho_{cg}\mathbf{C}_{cg})^{-1}\mathbf{M}_{cg} + \delta^2_{cg}\mathbf{I}$, which we optimized for $\boldsymbol{\theta}_{cg} = (\sigma^2_{cg}, \rho_{cg}, \delta^2_{cg})^T$. For $\boldsymbol{\Sigma}_{cg}$ to be positive definite, $\sigma^2_{cg} > 0$, $-1.104 < \rho_{cg} < 1.013$, and $\delta^2_{cg} \geq 0$. Because $\boldsymbol{\theta}_{cg} = (1, 1, 0)^T$ is in the parameter space, we can do no worse than the spherical geostatistical model. In fact, upon optimizing, we obtained $\mathcal{L}(\hat{\boldsymbol{\theta}}_{cg}|\mathbf{y}) = 373.95$, where $\hat{\sigma}^2_{cg} = 0.941$, $\hat{\rho}_{cg} = 1.01$, and $\hat{\delta}^2_{cg} = 0$, a slightly better optimization than the spherical geostatistical model. The marginal variances for this geostatistical-assisted CAR model are shown in Fig. 3d, and the marginal

correlations are shown in Fig. 4d. Note the rather large changes from Fig. 3c to Fig. 3d, and from Fig. 4c to Fig. 4d, with seemingly minor changes in $\hat{\sigma}^2_{cg}$, from 1 to 0.941, and in ρ_{cg}, from 1 to 1.01. Others have documented rapid changes in CAR model behavior near the parameter boundaries, especially for ρ_{cg} (Besag and Kooperberg, 1995; Wall, 2004). Note that for optimizing likelihoods, we transform ρ_{cg} with a logit so that it is unbounded, and scaled so that the inverse logit is between -1.104 and 1.013. On the logit-transformed scale, the rapid changes in ρ_{cg} near the bounds are no longer dramatic as they get stretched toward $-\infty$ and ∞.

5. Discussion and conclusions

Some detailed comparisons of the mathematical relationships between CAR and SAR models have been given in Besag (1974), Haining (1990, p. 89), and Cressie (1993, p. 408). Haining (1990, p. 89) provided several results that we restate using notation from Sections 2.1 and 2.2, and show that some are incorrect or incomplete.

In an attempt to create a CAR covariance matrix from a SAR covariance matrix, assume that $\mathbf{B}$ satisfies conditions S1–S3 and $\boldsymbol{\Omega} = \mathbf{I}$ in (2). Let $\mathbf{M} = \mathbf{I}$ and $\mathbf{C}$ be symmetric in (4) [which omits the important case (6)]. Then setting SAR and CAR covariances matrix equal to each other,

$$(\mathbf{I} - \mathbf{C})^{-1} = [(\mathbf{I} - \mathbf{B})(\mathbf{I} - \mathbf{B}^T)]^{-1} = (\mathbf{I} - \mathbf{B} - \mathbf{B}^T + \mathbf{B}\mathbf{B}^T)^{-1}, \tag{9}$$

and Haining (1990) claims that $\mathbf{C}$ can be obtained from $\mathbf{B}$ by setting

$$\mathbf{C} = \mathbf{B} + \mathbf{B}^T - \mathbf{B}\mathbf{B}^T, \tag{10}$$

which is repeated in texts by Waller and Gotway (2004, p. 372) and Schabenberger and Gotway (2005, p. 339), and in the literature (e.g., Dormann et al., 2007). However, aside from the lack of generality due to assumptions $\mathbf{M} = \mathbf{I}$, $\boldsymbol{\Omega} = \mathbf{I}$, and symmetric $\mathbf{C}$, we note that (10) is incomplete and too limiting to be useful, as given in the following remark.

Remark 1. C3 in Section 2.2 is not satisfied for $\mathbf{C}$ in (10) except when $\mathbf{B}$ contains all zeros.

Proof. Because $\mathbf{B}$ has zeros on the diagonal, $\mathbf{B} + \mathbf{B}^T$ will have zeros on the diagonal. Denote $\mathbf{b}_i$ as the ith row of $\mathbf{B}$. Then the ith diagonal element of $\mathbf{B}\mathbf{B}^T$ will be $\mathbf{b}_i\mathbf{b}_i^T$, which will be zero only if all elements of $\mathbf{b}_i$ are zero. Hence, $\mathbf{B} + \mathbf{B}^T - \mathbf{B}\mathbf{B}^T$ will have zeros on the diagonal only if $\mathbf{B}$ contains all zeros. □

In an attempt to create a SAR covariance matrix from a CAR covariance matrix, assume the same conditions as for (9), and that $\mathbf{C}$ satisfies conditions C1–C4. Let $(\mathbf{I} - \mathbf{C}) = \mathbf{S}\mathbf{S}^T$, where $\mathbf{S}$ is a Cholesky decomposition. Haining (1990) suggested $\mathbf{S} = \mathbf{I} - \mathbf{B}$ and setting $\mathbf{B}$ equal to $\mathbf{I} - \mathbf{S}$. However, this is incomplete because condition S3 in Section 2.1 will be satisfied only if $\mathbf{S}$ has all ones on the diagonal, which is also extremely limiting.

For another approach to relate SAR and CAR covariance matrices, Haining (1990) described the model $\mathbf{F}(\boldsymbol{Z} - \boldsymbol{\mu}) = \mathbf{H}\boldsymbol{\epsilon}$, where $\text{var}(\boldsymbol{\epsilon}) = \mathbf{V}$. Then $\text{E}((\boldsymbol{Z} - \boldsymbol{\mu})(\boldsymbol{Z} - \boldsymbol{\mu})^T) = \mathbf{F}^{-1}\mathbf{H}\mathbf{V}\mathbf{H}^T(\mathbf{F}^{-1})^T$. Now let $\mathbf{F} = (\mathbf{I} - \mathbf{C})$, $\mathbf{H} = \mathbf{I}$, and $\mathbf{V} = (\mathbf{I} - \mathbf{C})$ (this appears to originate in Martin (1987)). The constructed model is really a SAR model except that it violates condition S2 by allowing $\mathbf{V} = (\mathbf{I} - \mathbf{C})$. Alternatively, this can be seen as an attempt to create a SAR model from a CAR model by assuming an inverse CAR covariance matrix for the error structure of the SAR model, which gains nothing. Because these arguments are unconvincing, and other authors argue that one cannot go uniquely from a CAR to a SAR (e.g., Mardia, 1990), we can find no further citations for the arguments of Haining (1990) on obtaining a SAR covariance matrix from a CAR covariance matrix.

Besag (1974) provided a demonstration of how a SAR covariance matrix with first-order neighbors in $\mathbf{B}$ leads to a CAR covariance matrix with third-order neighbors in $\mathbf{C}$, which we reproduce here. Assume a rectangular lattice, as in Fig. 1a, but with all first order neighbors, and assume it is on a torus (making the top row neighbors of the bottom row, and the left side neighbors of the right side, so all sites have 4 neighbors. Let $Z_{i,j}$ be a random variable in the ith row and j column of the lattice. Assume a SAR model (2) with non-symmetric $\mathbf{B}$, created from

$$Z_{i,j} = \beta_1 Z_{i-1,j} + \beta_1' Z_{i+1,j} + \beta_2 Z_{i,j-1} + \beta_2' Z_{i,j-1} + \varepsilon_{i,j}, \tag{11}$$

where assume that var($\{\varepsilon_{i,j}\}$) $= \Omega = \mathbf{I}$. Then Besag (1974) showed that the corresponding CAR model is

$$\begin{aligned} E(Z_{i,j}|\{z_{k,\ell} : (k,\ell) \neq (i,j)\}) = (1 + \beta_1^2 + \beta_1'^2 + \beta_2^2 + \beta_2'^2)^{-1}\{&(\beta_1 + \beta_1')(z_{i-1,j} + z_{i+1,j}) \\ &+ (\beta_2 + \beta_2')(z_{i,j-1} + z_{i,j+1}) - (\beta_1\beta_2' + \beta_1'\beta_2)(z_{i-1,j-1} + z_{i-1,j+1}) \\ &- (\beta_1\beta_2 + \beta_1'\beta_2')(z_{i-1,j+1} + z_{i+1,j-1}) - (\beta_1\beta_1')(z_{i-2,j} + z_{i+2,j}) - (\beta_2\beta_2')(z_{i,j-2} + z_{i,j+2})\}, \end{aligned} \quad (12)$$

which follows by creating the covariance matrix from the SAR weights (11) and applying Theorem 2. Cressie (1993, p. 409) gave a version of (12) where $\mathbf{B}$ was symmetric, although his formula had terms in it with incorrect signs. Besag's result (12) is useful for its generality in either the symmetric or non-symmetric case. If all $\beta_1, \beta_1', \beta_2, \beta_2'$ are nonzero the first-order SAR (11) leads to third-order CAR weights (12). It appears that, generally, there will be no equivalent SAR covariance matrices for first and second-order CAR covariance matrices. However, consider setting $\beta_1' = \beta_2 = \beta_2' = 0$, in which case an asymmetric first-order SAR weighting leads to a first-order CAR matrix (although only for the row weightings). Moreover, our demonstration in Fig. 1c shows that a sparse $\mathbf{B}$ may be obtained from a sparse CAR model, although it is asymmetric and may not have the usual neighborhood interpretation.

There are other parameterizations for CAR models. In (6) and (7) we introduced parameterizations for a CAR model that can more generally be written as

$$\boldsymbol{\Sigma}_{\text{CAR}} = (\mathbf{D} - \mathbf{C}^{\#})^{-1},$$

where the diagonal elements of $\mathbf{C}^{\#}$ are zero, and $\mathbf{D}$ is diagonal. A reviewer pointed out that it is also useful to parameterize a CAR model as $\boldsymbol{\Sigma}_{\text{CAR}}^{-1} = \mathbf{C}^*$, in which case the conditional specification in terms of elements of $\mathbf{C}^*$ is

$$Z_i|\mathbf{z}_{-i} \sim N\left(-\sum_{j\neq i}\frac{c^*_{i,j}}{c^*_{i,i}}z_j, \frac{\sigma^2}{c^*_{i,i}}\right), \quad (13)$$

which can be compared to (3). Each parameterization has its virtues. The unscaled weights are given directly in (3) including a zero weight for Z_i. To build models, one could simply say that $\mathbf{C}^*$ must be positive definite, but more specific conditions on the diagonals and off-diagonals, similar to conditions C1–C4 in Section 2.2, are useful, as illustrated by the construction of weights in Section 2.3. On the other hand, we can go from a SAR covariance matrix to a CAR covariance matrix simply by using $\mathbf{C}^* = (\mathbf{I} - \mathbf{B})\Omega^{-1}(\mathbf{I} - \mathbf{B}^T)$. It is also easy to see from the proof of Theorem 1 that it is possible to obtain a non-unique SAR covariance matrix from $\mathbf{C}^*$, as we did for $\mathbf{C}$.

From Section 2.3, we showed that, for SAR models, pre-specified weights $\mathbf{B} = \rho\mathbf{W}$ are often scaled by ρ, and that ρ is often constrained by the eigenvalues of $\mathbf{W}$. However, we also discussed in Section 3.1 that weights can be chosen so that all eigenvalues are zero for SAR models. Fig. 1c provides an example where all diagonal elements of $\mathbf{B}$ are zero, and hence a SAR model where all eigenvalues of $\mathbf{B}$ are zero. We have little information or guidance for developing models where all eigenvalues of $\mathbf{B}$ are zero, and this provides an interesting topic for future research.

Wall (2004) provided a detailed comparison on properties of marginal correlation for various values of ρ when $\mathbf{B}$ or $\mathbf{C}$ are parameterized as $\rho_s\mathbf{W}$ and $\rho_c\mathbf{W}$, respectively, but did not develop mathematical relationships between CAR and SAR models. Lindgren et al. (2011) showed that approximations to point-referenced geostatistical models based on a finite element basis expansion can be expressed as CAR models. In his discussion of the same, Kent (2011) noted that, for a given geostatistical model of the Matern class, one could construct either a CAR or SAR model that would approximate the Matern model. This indicates a correspondence between CAR and SAR models when used as approximations to continuous-space processes, but does not address the relationship between CAR and SAR models on a native areal support.

Our literature review and discussion showed that there have been scattered efforts to establish mathematical relationships between CAR and SAR models, and some of the reported relationships are incomplete on the conditions for those relationships. With Theorems 1 and 2 and Corollary 1, we demonstrated that any zero-mean Gaussian distribution on a finite set of points, $\boldsymbol{Z} \sim \text{N}(\mathbf{0}, \boldsymbol{\Sigma})$, with positive-definite covariance matrix $\boldsymbol{\Sigma}$, can be written as either a CAR or a SAR model, with the important difference that a CAR model is uniquely determined from $\boldsymbol{\Sigma}$ but a SAR model is not so uniquely

determined. This equivalence between CAR and SAR models can also have practical applications. In addition to our examples, the full conditional form of the CAR model allows for easy and efficient Gibbs sampling (Banerjee et al., 2004, p. 163) and fully conditional random effects (Banerjee et al., 2004, p. 86). However, spatial econometricians often employ SAR models (LeSage and Pace, 2009), so easy conversion from SAR to CAR models may offer computational advantages in hierarchical models and provide insight on the role of fully conditional random effects. We expect future research will extend our findings on relationships between CAR and SAR models and explore novel applications.

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Appendix. Propositions and proofs

The following proposition is used to show condition C1 for CAR models.

Proposition 1. *For the CAR model covariance matrix,* $\boldsymbol{\Sigma}_{CAR} = (\mathbf{I} - \mathbf{C})^{-1}\mathbf{M}$ *in (4),* $\boldsymbol{\Sigma}_{CAR}$ *is positive definite if and only if all eigenvalues of* $(\mathbf{I} - \mathbf{C})$ *are positive.*

Proof. Note that $\mathbf{I} - \mathbf{M}^{-1/2}\mathbf{C}\mathbf{M}^{1/2}$ will be symmetric because of condition C4, and hence will have real eigenvalues. Write $\boldsymbol{\Sigma}_{\text{CAR}}{}^{-1} = \mathbf{M}^{-1/2}(\mathbf{I} - \mathbf{M}^{-1/2}\mathbf{C}\mathbf{M}^{1/2})\mathbf{M}^{-1/2}$. Then $\boldsymbol{\Sigma}_{\text{CAR}}$ and $\boldsymbol{\Sigma}_{\text{CAR}}{}^{-1}$ are positive definite if and only if $\mathbf{I} - \mathbf{M}^{-1/2}\mathbf{C}\mathbf{M}^{1/2}$ is positive definite, i.e., if and only if all eigenvalues of $(\mathbf{I} - \mathbf{M}^{-1/2}\mathbf{C}\mathbf{M}^{1/2})$ are positive. Now, $(\mathbf{I} - \mathbf{C}) = \mathbf{M}^{1/2}(\mathbf{I} - \mathbf{M}^{-1/2}\mathbf{C}\mathbf{M}^{1/2})\mathbf{M}^{-1/2}$ has positive eigenvalues if and only if $(\mathbf{I} - \mathbf{M}^{-1/2}\mathbf{C}\mathbf{M}^{1/2})$ has positive eigenvalues because they are similar matrices (Harville, 1997, p. 525). □

Next, we show the conditions on ρ that ensure that $(\mathbf{I} - \rho\mathbf{W})$ has either nonzero eigenvalues, or positive eigenvalues.

Proposition 2. *Consider the* $N \times N$ *matrix* $(\mathbf{I} - \rho\mathbf{W})$*, where* $w_{i,i} = 0$*. Let* $\{\lambda_i\}$ *be the set of eigenvalues of* $\mathbf{W}$*, and suppose all eigenvalues are real. Then*

(i) $\mathbf{I} - \rho\mathbf{W}$ *is nonsingular if and only if* $\rho \notin \{\lambda_i^{-1}\}$ *for all nonzero* λ_i*.*
(ii) *Assume at least two eigenvalues of* $\mathbf{W}$ *are nonzero, and let* $\lambda_{[1]}$ *and* $\lambda_{[N]}$ *be the smallest and largest eigenvalues, respectively, of* $\mathbf{W}$*. Then all eigenvalues of* $\mathbf{I} - \rho\mathbf{W}$ *are positive if and only if* $1/\lambda_{[1]} < \rho < 1/\lambda_{[N]}$*.*

Proof. Let λ_i be an eigenvalue of $\mathbf{W}$, with $\mathbf{v}_i$ a corresponding eigenvector. Then $\mathbf{W}\mathbf{v}_i = \lambda_i\mathbf{v}_i$, implying that $\mathbf{v}_i - \rho\mathbf{W}\mathbf{v}_i = \mathbf{v}_i - \rho\lambda_i\mathbf{v}_i = (1 - \rho\lambda_i)\mathbf{v}_i$, i.e., $(\mathbf{I} - \rho\mathbf{W})\mathbf{v}_i = (1 - \rho\lambda_i)\mathbf{v}_i$. Thus, for every eigenvalue/eigenvector pair $(\lambda_i, \mathbf{v}_i)$ of $\mathbf{W}$, there is a corresponding eigenvalue/eigenvector pair $(\omega_i, \mathbf{v}_i)$ of $(\mathbf{I} - \rho\mathbf{W})$ where $\omega_i = 1 - \rho\lambda_i$. Observe that $\mathbf{I} - \rho\mathbf{W}$ is nonsingular if and only if all $\omega_i \neq 0$, i.e., if and only if $\rho\lambda_i \neq 1$ for all i, i.e., if and only if $\rho \neq 1/\lambda_i$ for all nonzero λ_i. This establishes part (i). Furthermore, all eigenvalues of $\mathbf{I} - \rho\mathbf{W}$ are positive if and only if $\rho\lambda_i < 1$ for all i, i.e., if and only if $\rho < 1/\lambda_i$ for all i such that $\lambda_i > 0$, $\rho > 1/\lambda_i$ for all i such that $\lambda_i < 0$, and $\rho \in (-\infty, \infty)$ for all i such that $\lambda_i = 0$. This last set of three conditions can be restated as $1/\lambda_{[1]} < \rho < 1/\lambda_{[N]}$, which establishes part (ii). □

For CAR models (4), Cressie and Chan (1989) consider the symmetric matrix $\mathbf{M}^{-1/2}\mathbf{W}\mathbf{M}^{1/2}$ and (see Cressie, 1993, p. 559) shows bounds on ρ for $\mathbf{I} - \rho\mathbf{M}^{-1/2}\mathbf{W}\mathbf{M}^{1/2}$ so that all eigenvalues are positive. Here, we state the proposition without proof, as it proceeds in a similar fashion to Proposition 2.

Proposition 3. *Consider the $N \times N$ matrix $(\mathbf{I} - \rho\mathbf{M}^{-1/2}\mathbf{W}\mathbf{M}^{1/2})$, where $w_{i,i} = 0$ and $\mathbf{M}$ is diagonal with positive values such that $\mathbf{M}^{-1/2}\mathbf{W}\mathbf{M}^{1/2}$ is symmetric with eigenvalues $\{\lambda_i\}$. Then*

(i) $\mathbf{I} - \rho\mathbf{M}^{-1/2}\mathbf{W}\mathbf{M}^{1/2}$ *is nonsingular if and only if* $\rho \notin \{\lambda_i^{-1}\}$ *for all nonzero* λ_i.
(ii) *Assume at least two eigenvalues of* $\mathbf{M}^{-1/2}\mathbf{W}\mathbf{M}^{1/2}$ *are nonzero, and let* $\lambda_{[1]}$ *and* $\lambda_{[N]}$ *be the smallest and largest eigenvalues, respectively, of* $\mathbf{M}^{-1/2}\mathbf{W}\mathbf{M}^{1/2}$. *Then all eigenvalues of* $\mathbf{I} - \rho\mathbf{M}^{-1/2}\mathbf{W}\mathbf{M}^{1/2}$ *are positive if and only if* $1/\lambda_{[1]} < \rho < 1/\lambda_{[N]}$.

While this result was developed for CAR models, note that these bounds would also work for a SAR covariance matrix (2) if $\boldsymbol{\Omega}$ had diagonal elements such that $\boldsymbol{\Omega}^{-1/2}\mathbf{W}\boldsymbol{\Omega}^{1/2}$ was symmetric (Wall, 2004). Before proving Theorems 1 and 2, some preliminary results are useful.

Proposition 4. *If* $\mathbf{D}$ *is a diagonal matrix and* $\mathbf{Q}$ *is a square matrix with zeros on the diagonal of the same dimensions as* $\mathbf{D}$, *then both* $\mathbf{DQ}$ *and* $\mathbf{QD}$ *have zeros on the diagonal.*

Proof. We omit the proof because it is apparent from the algebra of matrix products. □

Proposition 5. *Let* $\mathbf{A}$, $\mathbf{B}$, *and* $\mathbf{C}$ *be square matrices. If* $\mathbf{A} = \mathbf{BC}$, *and* $\mathbf{A}$ *and* $\mathbf{C}$ *have inverses, then* $\mathbf{B}$ *has an inverse.*

Proof. Because $\mathbf{C}$ has an inverse, $\mathbf{B} = \mathbf{AC}^{-1}$, and because $\mathbf{A}$ has an inverse, $\mathbf{B}^{-1} = \mathbf{CA}^{-1}$. □

Finally, we show the proofs of Theorems 1 and 2.

Theorem 1. *Any positive definite covariance matrix* $\boldsymbol{\Sigma}$ *can be expressed as the covariance matrix of a SAR model* $(\mathbf{I} - \mathbf{B})^{-1}\boldsymbol{\Omega}(\mathbf{I} - \mathbf{B}^T)^{-1}$, (2), *for a (non-unique) pair of matrices* $\mathbf{B}$ *and* $\boldsymbol{\Omega}$.

Proof. We consider a constructive proof and show that the matrices $\mathbf{B}$ and $\boldsymbol{\Omega}$ that we construct satisfy conditions S1–S3.

(i) Since $\boldsymbol{\Sigma}$ is positive definite, so is $\boldsymbol{\Sigma}^{-1}$ and we may write $\boldsymbol{\Sigma}^{-1} = \mathbf{LL}^T$ where $\mathbf{L}$ is full rank with positive diagonal elements. Note that $\mathbf{L}$ is *not* unique. A Cholesky decomposition (Harville, 1997, p. 229) could be used, where $\mathbf{L}$ is lower triangular, or a spectral (eigen) decomposition could be used to obtain a square-root matrix (Harville, 1997, p. 543), where $\boldsymbol{\Sigma}^{-1} = \mathbf{VEV}^T$, with $\mathbf{V}$ containing orthonormal eigenvectors and $\mathbf{E}$ containing eigenvalues on the diagonal and zeros elsewhere. Then $\mathbf{L} = \mathbf{VE}^{1/2}\mathbf{V}^T$ is symmetric with positive diagonal elements, where the diagonal matrix $\mathbf{E}^{1/2}$ contains the positive square roots of the eigenvalues in $\mathbf{E}$.
(ii) Decompose $\mathbf{L}$ into $\mathbf{L} = \mathbf{G} - \mathbf{P}$ where $\mathbf{G}$ is diagonal and $\mathbf{P}$ has zeros on the diagonal. Then $\mathbf{LL}^T = (\mathbf{G} - \mathbf{P})(\mathbf{G}^T - \mathbf{P}^T)$ by construction.
(iii) Then set

$$\boldsymbol{\Omega}^{-1} = \mathbf{GG} \text{ and } \mathbf{B}^T = \mathbf{PG}^{-1}. \tag{A.1}$$

Note that because $\mathbf{L}$ has positive diagonal elements, then $\ell_{i,i} > 0$, and because $\mathbf{G}$ is diagonal with $g_{i,i} = \ell_{i,i}$, $\mathbf{G}^{-1}$ exists.

Then $\boldsymbol{\Sigma}^{-1} = (\mathbf{I} - \mathbf{B}^T)\boldsymbol{\Omega}^{-1}(\mathbf{I} - \mathbf{B})$, expressed in SAR form (2). The matrices $\mathbf{B}$ and $\boldsymbol{\Omega}$ satisfy S1–S3, as follows.

(S1) Note that $\mathbf{P} = \mathbf{B}^T\mathbf{G}$, so $\mathbf{L} = \mathbf{G} - \mathbf{P} = (\mathbf{I} - \mathbf{B}^T)\mathbf{G}$ and $\mathbf{L}^T = \mathbf{G}(\mathbf{I} - \mathbf{B})$. Then, by Proposition 5, $(\mathbf{I} - \mathbf{B})^{-1}$ exists, and hence so does its transpose $(\mathbf{I} - \mathbf{B}^T)^{-1}$.
(S2) Because $\mathbf{G}$ is diagonal, $\boldsymbol{\Omega}$ is diagonal with $\omega_{i,i} = g_{i,i}^2 > 0$.
(S3) By Proposition 4, $b_{i,i} = 0$ because $\mathbf{B}^T = \mathbf{PG}^{-1}$. □

Theorem 2. *Any positive-definite covariance matrix* $\boldsymbol{\Sigma}$ *can be expressed as the covariance matrix of a CAR model* $(\mathbf{I} - \mathbf{C})^{-1}\mathbf{M}$, (4), *for a unique pair of matrices* $\mathbf{C}$ *and* $\mathbf{M}$.

Proof. We add an explicit, constructive proof of the result given by Cressie and Wikle (2011, p. 185–186) by showing that matrices $\mathbf{C}$ and $\mathbf{M}$ are unique and satisfy conditions C1–C4.

(i) Let $\mathbf{Q} = \boldsymbol{\Sigma}^{-1}$ and decompose it into $\mathbf{Q} = \mathbf{D} - \mathbf{R}$, where $\mathbf{D}$ is diagonal with elements $d_{i,i} = q_{i,i}$ (the diagonal elements of the precision matrix $\mathbf{Q}$), and $\mathbf{R}$ has zeros on the diagonal ($r_{i,i} = 0$) and off-diagonals equal to $r_{i,j} = -q_{i,j}$.

(ii) Set

$$\mathbf{C} = \mathbf{D}^{-1}\mathbf{R} \text{ and } \mathbf{M} = \mathbf{D}^{-1}. \tag{A.2}$$

Then $\boldsymbol{\Sigma}^{-1} = \mathbf{D} - \mathbf{R} = \mathbf{D}(\mathbf{I} - \mathbf{D}^{-1}\mathbf{R}) = \mathbf{M}^{-1}(\mathbf{I} - \mathbf{C})$, which shows that $\boldsymbol{\Sigma}$ may be expressed in CAR form (4), satisfying C1–C4.

(C1) $\mathbf{M}$ is strictly diagonal with positive values, so $\mathbf{M}$ and $\mathbf{M}^{-1}$ are positive definite. By hypothesis, $\boldsymbol{\Sigma}$, and hence $\boldsymbol{\Sigma}^{-1}$, are positive definite. Then $\boldsymbol{\Sigma} = (\mathbf{I} - \mathbf{C})^{-1}\mathbf{M}$, so by Proposition 1, $(\mathbf{I} - \mathbf{C})^{-1}$ has positive eigenvalues and thus so does $\mathbf{I} - \mathbf{C}$.

(C2) $m_{i,i} = 1/q_{i,i}$, and because $\mathbf{Q} = \boldsymbol{\Sigma}^{-1}$ is positive definite, we have that $q_{i,i} > 0$, $i = 1, 2, \ldots, n$. Thus, each $m_{i,i} > 0$. By construction, $m_{i,j} = 0$ for $i \neq j$.

(C3) By Proposition 4, $c_{i,i} = 0$ because $\mathbf{C} = \mathbf{D}^{-1}\mathbf{R}$.

(C4) For $i \neq j$, we have that $c_{i,j} = d_{i,i}^{-1} r_{i,j}$. As $m_{i,i} = d_{i,i}^{-1}$, we have that

$$\frac{c_{i,j}}{m_{i,i}} = \frac{d_{i,i}^{-1} r_{i,j}}{d_{i,i}^{-1}} = r_{i,j} = -q_{i,j}.$$

Because $\mathbf{Q} = \boldsymbol{\Sigma}^{-1}$ is symmetric, $q_{i,j} = q_{j,i}$, hence $c_{i,j}/m_{i,i} = c_{j,i}/m_{j,j}$. The above proof shows existence of a CAR representation of any covariance matrix $\boldsymbol{\Sigma}$. We now show uniqueness of this CAR representation. Assume that there exists $\tilde{\mathbf{C}}$ and $\tilde{\mathbf{M}}$, possibly different from $\mathbf{C}$ and $\mathbf{M}$ in (A.2)), that satisfy C1–C4, and also satisfy $\boldsymbol{\Sigma} = \tilde{\mathbf{M}}^{-1}(\mathbf{I} - \tilde{\mathbf{C}})$. From Proposition 4, we have that $\mathrm{diag}(\mathbf{M}) = \mathrm{diag}(\tilde{\mathbf{M}}) = \mathrm{diag}(\boldsymbol{\Sigma}^{-1})$, and so $\mathbf{M} = \tilde{\mathbf{M}}$, since $\mathbf{M}$ and $\tilde{\mathbf{M}}$ are diagonal matrices. Furthermore, since $\mathbf{M}^{-1}(\mathbf{I} - \mathbf{C}) = \boldsymbol{\Sigma} = \tilde{\mathbf{M}}^{-1}(\mathbf{I} - \tilde{\mathbf{C}})$, we have that $\tilde{\mathbf{C}} = \mathbf{I} - \tilde{\mathbf{M}}\mathbf{M}^{-1}(\mathbf{I} - \mathbf{C})$, but since $\mathbf{M} = \tilde{\mathbf{M}}$, it immediately follows that $\mathbf{C} = \tilde{\mathbf{C}}$, and we thus conclude that the CAR representation of $\boldsymbol{\Sigma}$ is unique. □

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