

**Handout 4: Aerial unit data / spatial data on lattices**

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**Aim.** To introduce Aerial unit data modeling: the basic building models.**Reading list & references:**

- [1] Cressie, N. (2015; Part II). Statistics for spatial data. John Wiley & Sons.
- [2] Gaetan, C., & Guyon, X. (2010; Ch 3). Spatial statistics and modeling (Vol. 90). New York: Springer.

**Specialized reading.**

- [3] Kent, J. T., & Mardia, K. V. (2022). Spatial analysis (Vol. 72). John Wiley & Sons. (on Spatial analysis)

**Part 1. Basic stochastic models & related concepts for model building**

*Note 1.* Recall from Section 2.2 of “Handout 1: Types of spatial data” that modeling aerial unit / lattice data types involves the use of random field models with a discrete index set. Such data are collected over areal units such as pixels, census districts or tomographic bins. Often, there is a natural neighborhood relation or neighborhood structure.

*Note 2.* This means we need to introduce suitable basic building models able to represent the characteristics of the underline data generating mechanisms. These as the “Discrete Random Fields”.

**1. DISCRETE RANDOM FIELDS**

*Note 3.* We re-introduce the definition of the random field with regards to the aerial unit data framework.

**Definition 4.** A random field  $Z = (Z_s; s \in \mathcal{S})$  on a set of indexes  $\mathcal{S}$  taking values in  $\mathcal{Z}^{\mathcal{S}}$  is a family of random variables  $\{Z_s := Z_s(\omega); s \in \mathcal{S}, \omega \in \Omega\}$  where each  $Z_s(\omega)$  is defined on the same probability space  $(\Omega, \mathfrak{F}, \text{pr})$  and taking values in  $\mathcal{Z}$ .

*Note 5.* In aerial unite data modeling, the (spatial) set of sites  $\mathcal{S}$ , at which the process is defined, is discrete, it can be finite or infinite (e.g.  $\mathcal{S} \subseteq \mathbb{Z}^d$ ), regular (e.g. pixels of an image) or irregular (states of a country).

*Note 6.* The general state space  $\mathcal{Z}$  of the random field can be quantitative, qualitative or mixed. E.g.,  $\mathcal{Z} = \mathbb{R}_+$  in a Gamma random field,  $\mathcal{Z} = \mathbb{N}$  in a Poisson random field,  $\mathcal{Z} = \{0, 1\}$  in a binary random field.

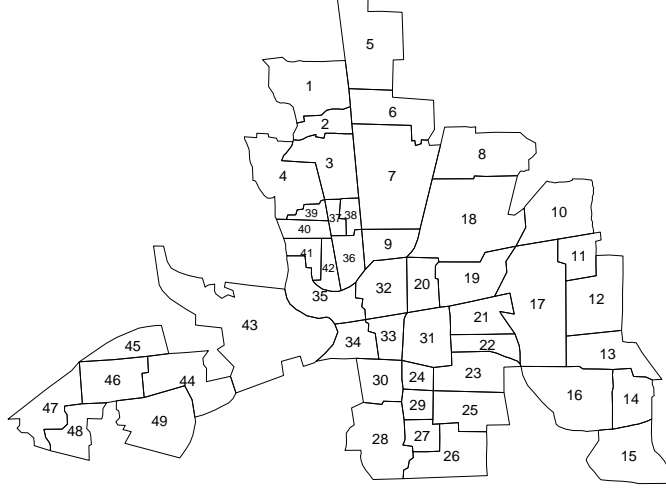


FIGURE 1.1. Lattice of spatial sites for Columbus dataset. Each neighborhood is a site. Each site is labeled. The collection of sites is the lattice of sites.

*Note 7.* If  $\mathcal{Z}$  is finite or countably infinite, the (joint)distribution of  $Z$  has a PMF

$$\text{pr}_Z(z) = \text{pr}(Z = z) = \text{pr}(\{Z_s = z_s; s \in \mathcal{S}\}), \forall z \in \mathcal{Z}^{\mathcal{S}}$$

otherwise if  $\mathcal{Z} \subseteq \mathbb{R}^d$  and  $Z$  continuous we will use the joint PDF.

**Definition 8.** The discrete set of sites  $\mathcal{S} = \{s_i; i = 1, \dots, n\}$  is often called lattice of sites.

*Notation 9.* More often we will use the notation  $Z_s$  instead of  $Z(s)$  or  $Z_i$  instead of  $Z(s_i)$ . Hence, since  $\mathcal{S} = \{s_i; i = 1, \dots, n\}$ , we can consider a more convenient notation

$$Z = (Z_s; s \in \mathcal{S})^\top = (Z_i = Z(s_i); i = 1, \dots, n)^\top.$$

*Notation 10.* The notation  $i \sim j$  between two sites  $i, j \in \mathcal{S}$  means that “sites  $i$  and  $j$  are neighboring” according to a “neighborhood relation”  $\sim$ .

**Example 11.** Consider the Columbus OH dataset which concerns spatially correlated count data arising from 49 districts/neighborhood in Columbus, OH in 1980. This is the R dataset `columbus{spdep}`. Figure 1.1 presents the sites and the lattice of sites. Each neighborhood is a site. Each site is label. The collection of sites is the lattice of sites coded with a unique labeled according to some order. One may define the “neighborhood relation  $i \sim j$  considering counties that share common borders (adjacent). Then for site  $i = 43$ ,  $i \sim j$  involves any  $j \in \{44, 35, 34\}$  and for site  $i = 20$ ,  $i \sim j$  involves any  $j \in \{32, 9, 18, 19, 31, 33\}$ .

**Example 12.** (Logistic/Ising model) Let variable  $Z_i$  denote the presence of a characteristic as  $Z_i = 1$  or absence of it as  $Z_i = 0$  on a site labeled by  $i \in \mathcal{S}$ . Then  $\mathcal{Z} = \{0, 1\}$ . The Ising

model is defined by the (joint) PMF

$$(1.1) \quad \text{pr}_Z(z) \propto \exp \left( \alpha \sum_{i \in \mathcal{S}} z_i + \beta \sum_{\{i,j\}: i \sim j} z_i z_j \right), \quad \forall z \in \mathcal{Z}^{\mathcal{S}}$$

E.g., it can model a black & white noisy image, where  $\mathcal{S}$  denotes the labels of the image pixels, and  $Z_i$  denotes the presence of a black pixel ( $Z_i = 1$ ) or its absence ( $Z_i = 0$ ). Under Ising model (1.1), the characteristic is observed with probability  $\text{pr}_{Z_i}(z_i = 1) = \frac{\exp(\alpha)}{1 + \exp(\alpha)}$  when  $\beta = 0$ . The characteristic's presence is encouraged in neighboring sites when  $\beta > 0$ , and discouraged when  $\beta < 0$ .

*Notation 13.* We use notation, for  $\mathcal{A} \subset \mathcal{S}$

$$\text{pr}_{\mathcal{A}}(z_{\mathcal{A}} | z_{\mathcal{S} \setminus \mathcal{A}}) = \text{pr}(Z_{\mathcal{A}} = z_{\mathcal{A}} | Z_{\mathcal{S} \setminus \mathcal{A}} = z_{\mathcal{S} \setminus \mathcal{A}})$$

**Definition 14.** Local characteristics of a random field  $Z$  on  $\mathcal{S}$  with values in  $\mathcal{Z}$  are the conditionals

$$\text{pr}_i(z_i | z_{\mathcal{S} - i}) = \text{pr}_{\{i\}}(z_{\{i\}} | z_{\mathcal{S} \setminus \{i\}}), \quad i \in \mathcal{S}, z \in \mathcal{Z}$$

**Example 15.** (Cont. Example 12) The local characteristics of the Ising model in (1.1) are

$$\text{pr}_i(z_i = 1 | z_{\mathcal{S} - i}) = \frac{\exp \left( \alpha + \beta \sum_{\{i,j\}: i \sim j} z_j \right)}{1 + \exp \left( \alpha + \beta \sum_{\{i,j\}: i \sim j} z_j \right)}$$

## 2. COMPATIBILITY OF CONDITIONAL DISTRIBUTIONS

*Note 16.* Here, we discuss how to represent a joint probability distribution via its full conditionals. We need this for model building purposes.

**Definition 17.** Let random vector  $Z = (Z_1, \dots, Z_n)$  with joint distribution  $\pi(Z_1, \dots, Z_n)$ . The set of distributions  $\{\pi_i(\cdot | Z_{-i}); i = 1, \dots, n\}$  is called compatible to the joint distribution  $\pi(Z_1, \dots, Z_n)$  if the joint distribution  $\pi(Z_1, \dots, Z_n)$  has conditionals  $\{\pi_i(Z_i | Z_{-i}); i = 1, \dots, n\}$ .

*Note 18.* To specify suitable building models representing spatial dependency of a random field  $(Z_i)_{i \in \mathcal{S}}$ , it is often easier to visualize the joint distribution  $\text{pr}_z$  in terms of conditional distributions  $\{\pi_i(Z_i | Z_{\mathcal{S} - i}); i \in \mathcal{S}\}$  rather than directly.

*Note 19.* Thus, instead of specifying a joint model for  $(Z_i)_{i \in \mathcal{S}}$ , a researcher may propose putative families of conditional distributions  $\{\pi_i(Z_i | Z_{\mathcal{S} - i}); i \in \mathcal{S}\}$ . However, an arbitrary chosen set of conditional distributions  $\{\pi_i(\cdot | \cdot); i \in \mathcal{S}\}$  is not generally compatible, in the sense that there exists a joint distribution for  $(Z_i)_{i \in \mathcal{S}}$ , and hence we need to impose conditions.

*Note 20.* In what follows, we discuss necessary and sufficient conditions regarding compatibility.

**Proposition 21.** (Compatibility condition) Let  $F$  be a joint distribution with  $dF(x, y) = f(x, y) d(x, y)$  on  $\mathcal{S}_x \times \mathcal{S}_y$ . Let candidate condition distributions

$$G \text{ with } dG(x|y) = g(x|y) dx, \text{ on } x \in \mathcal{S}_x$$

$$Q \text{ with } dQ(y|x) = q(y|x) dy, \text{ on } y \in \mathcal{S}_y$$

and let  $N_g = \{(x, y) : g(x|y) > 0\}$  and  $N_q = \{(x, y) : q(y|x) > 0\}$ . A distribution  $F$  with conditionals exists iff

$$(1) N_g = N_q = N$$

$$(2) \text{ there exist functions } u \text{ and } v \text{ where } g(x|y)/q(y|x) = u(x)v(y) \text{ for all } (x, y) \in N \text{ and } \int u(x) dx < \infty$$

*Proof.* Omitted<sup>1</sup>. □

*Note 22.* Essentially the above conditions guarantee that

$$k(y) g(x|y) = f(x, y) = h(x) q(y|x)$$

where  $k, g, h, q$  are densities.

**Example 23.** The conditionals  $x|y \sim N(a + by, \sigma^2 + \tau^2 y^2)$  and  $y|x \sim N(c + dx, \tilde{\sigma}^2 + \tilde{\tau}^2 x^2)$  are compatible if  $\tau^2 = \tilde{\tau}^2 = 0$ ,  $d/\tilde{\sigma}^2 = b/\sigma^2$ , and  $|db| < 1$ .

**Solution.** See Exercise 23 in the Exercise sheet.

*Note 24.* Proposition 21 can be extended to more dimensions. For more info see (Arnold, B. C., & Press, S. J. (1989). in footnote 1)

*Note 25.* The following theorem shows that local characteristics can determine the entire distribution in certain cases.

**Theorem 26.** (Besag's factorization theorem; Brook's Lemma) Let  $Z$  be a  $\mathcal{Z}$  valued random field taking values in  $\mathcal{Z}^{\mathcal{S}}$  where  $\mathcal{S} = \{1, \dots, n\}$  with  $n \in \mathbb{N}$ , and such as  $pr_Z(z) > 0, \forall z \in \mathcal{Z}^{\mathcal{S}}$ . Then for all

$$(2.1) \quad \frac{pr_Z(z)}{pr_Z(z^*)} = \prod_{i=1}^n \frac{pr_i(z_i|z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)}{pr_i(z_i^*|z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)}, \quad \forall z, z^* \in \mathcal{Z}^{\mathcal{S}}$$

*Proof.* I will show that

$$pr_Z(z) = \prod_{i=1}^n \frac{pr_i(z_i|z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)}{pr_i(z_i^*|z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)} pr_Z(z^*)$$

<sup>1</sup>See Arnold, B. C., & Press, S. J. (1989). Compatible conditional distributions. Journal of the American Statistical Association, 84(405), 152-156.

It is

$$\text{pr}_Z(z_1, \dots, z_n) = \frac{\text{pr}_n(z_n | z_1, \dots, z_{n-2}, z_{n-1})}{\text{pr}_n(z_n^* | z_1, \dots, z_{n-2}, z_{n-1})} \text{pr}_Z(z_1, \dots, z_{n-1}, z_n^*)$$

Let proposition  $P_j$  be

$$\text{pr}_Z(z) = \prod_{i=n-j}^n \frac{\text{pr}_i(z_i | z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)}{\text{pr}_i(z_i^* | z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)} \text{pr}_Z(z_1, \dots, z_{n-j-1}, z_{n-j}^*, \dots, z_n^*)$$

Proposition  $P_0$  is true

$$(2.2) \quad \text{pr}_Z(z) = \frac{\text{pr}_n(z_n | z_1, \dots, z_{n-1})}{\text{pr}_n(z_n^* | z_1, \dots, z_{n-1})} \text{pr}_Z(z_1, \dots, z_{n-1}, z_n^*)$$

Proposition  $P_1$  is true

$$\text{pr}_Z(z_1, \dots, z_{n-1}, z_n^*) = \frac{\text{pr}_{n-1}(z_{n-1} | z_1, \dots, z_{n-2}, z_n^*)}{\text{pr}_{n-1}(z_{n-1}^* | z_1, \dots, z_{n-2}, z_n^*)} \text{pr}_Z(z_1, \dots, z_{n-2}, z_{n-1}^*, z_n^*)$$

Assume that  $P_j$  is true. Then proposition  $P_{j+1}$  is true as well, because

$$\begin{aligned} \text{pr}_Z(z) &= \prod_{i=n-j}^n \frac{\text{pr}_i(z_i | z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)}{\text{pr}_i(z_i^* | z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)} \text{pr}_Z(z_1, \dots, z_{n-j-1}, z_{n-j}^*, \dots, z_n^*) \\ &= \prod_{i=n-j}^n \frac{\text{pr}_i(z_i | z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)}{\text{pr}_i(z_i^* | z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)} \\ &\quad \times \frac{\text{pr}_{n-j-1}(z_{n-j-1} | z_1, \dots, z_{n-j-2}, z_{n-j}^*, \dots, z_n^*)}{\text{pr}_{n-j-1}(z_{n-j-1}^* | z_1, \dots, z_{n-j-2}, z_{n-j}^*, \dots, z_n^*)} \text{pr}_Z(z_1, \dots, z_{n-j-2}, z_{n-j-1}^*, \dots, z_n^*) \\ &= \prod_{i=n-(j+1)}^n \frac{\text{pr}_i(z_i | z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)}{\text{pr}_i(z_i^* | z_1, \dots, z_{i-1}, z_{i+1}^*, \dots, z_n^*)} \text{pr}_Z(z_1, \dots, z_{n-(j+1)-1}, z_{n-(j+1)}^*, \dots, z_n^*) \end{aligned}$$

Then (2.1) is correct according to the induction principle.  $\square$

*Note 27.* Theorem 26 shows that the joint  $\text{pr}_Z(\cdot)$  can be constructed from its conditionals  $\{\text{pr}_i(\cdot | \cdot)\}$  if distributions  $\{\text{pr}_i(\cdot | \cdot)\}$  are compatible for  $\text{pr}_Z(\cdot)$ , under the requirement that this construction is invariant wrt the coordinate permutation  $\{1, \dots, n\}$  and the reference state  $z^*$ — these invariances correspond to the conditions in Proposition 21.

### 3. GAUSSIAN AUTOREGRESSIVE MODELS

We present two basic spatial models, the CAR and SAR, able to represent spatial dependency.

**Definition 28.** Adjacency matrix  $N$  is called a matrix  $N$  with  $[N]_{i,j} = 1$  ( $i \sim j$ ) (it is implied that  $[N]_{i,i} = 0$ ) for some symmetric neighborhood relation  $\sim$  on  $\mathcal{S}$ . It aims at spatially connecting unites  $i$  and  $j$ .

**Definition 29.** Proximity matrix  $W$  is called a matrix  $W$  which aims at spatially connecting unites  $i$  and  $j$  in some fashion for some symmetric neighbourhood relation  $\sim$  on  $\mathcal{S}$ . Usually  $[W]_{i,i} = 0$

### 3.1. Conditional autoregressive models (CAR).

**Definition 30.** “Gaussian” Conditional autoregressive model, CAR, assumes that the local characteristics  $\{\text{pr}_i(z_i|z_{\mathcal{S}-i})\}$  are Gaussian distributions with mean  $E(Z_i|Z_{\mathcal{S}-i}) = \mu_i + \sum_{j \neq i} b_{i,j}(Z_j - \mu_j)$  and variance  $\text{Var}(Z_i|Z_{\mathcal{S}-i}) = \kappa_i$  for  $i \in \mathcal{S}$ ;

$$(3.1) \quad Z_i|z_{\mathcal{S}-i} \sim N\left(\mu_i + \sum_{j \neq i} b_{i,j}(Z_j - \mu_j), \kappa_i\right), \quad \forall i \in \mathcal{S}$$

**Proposition 31.** Let  $K = \text{diag}(\{\kappa_i\})$  with  $\kappa_i > 0$ , matrix  $B$  with  $B_{i,i} := [B]_{i,i} = 0$ , and real vector  $\mu$  with suitable dimensions. If  $Z$  follows a Gaussian CAR (Definition 30),  $I - B$  is non-singular, and  $(I - B)^{-1}K > 0$ , then the joint distribution of  $Z$  is

$$(3.2) \quad Z \sim N(\mu, (I - B)^{-1}K).$$

*Proof.* Without lose of generality, consider zero mean  $\mu = 0$  (or equivalently set  $Z := Z - \mu$ ). The full conditionals  $Z_i|z_{\mathcal{S}-i}$  in (3.1) are compatible with the joint distribution  $\text{pr}_Z(z)$ . By using Besag’s factorization theorem (Theorem 26) with reference state/configuration  $z^* = 0$  we get

$$\begin{aligned} \text{pr}_Z(z) &= \prod_{i=1}^n \frac{\text{pr}_i(z_i|z_1, \dots, z_{i-1}, z_{i+1}^* = 0, \dots, z_n^* = 0)}{\text{pr}_i(z_i^* = 0|z_1, \dots, z_{i-1}, z_{i+1}^* = 0, \dots, z_n^* = 0)} \text{pr}_Z(z^* = 0) \\ &= \prod_{i=1}^n \frac{N(z_i | \sum_{j < i} b_{i,j}z_j + 0, \kappa_i)}{N(0 | \sum_{j < i} b_{i,j}z_j + 0, \kappa_i)} \text{pr}_Z(z^* = 0) \\ &\propto \prod_{i=1}^n \exp\left(-\frac{1}{2\kappa_i} \left(z_i - \sum_{j < i} b_{i,j}z_j\right)^2 + \frac{1}{2\kappa_i} \left(0 - \sum_{j < i} b_{i,j}z_j\right)^2\right) \\ &= \prod_{i=1}^n \exp\left(-\frac{1}{2\kappa_i} \left(z_i^2 - 2z_i \sum_{j < i} b_{i,j}z_j\right)\right) \text{pr}_Z(z^* = 0) \\ &= \exp\left(-\sum_i \frac{z_i^2}{2\kappa_i} + \frac{1}{2} \sum_i \sum_{j < i} \frac{b_{i,j}}{\kappa_i} z_i z_j\right) \text{pr}_Z(z^* = 0) \\ &= \exp\left(-\frac{1}{2} z^\top K^{-1} z + \frac{1}{2} z^\top K^{-1} B z\right) \text{pr}_Z(z^* = 0) = \exp\left(-\frac{1}{2} z^\top [K^{-1}(I - B)] z\right) \text{pr}_Z(z^* = 0) \\ (3.3) \quad &= N(z|0, (I - B)^{-1}K) \end{aligned}$$

Recovering the mean from (3.3), it is

$$\text{pr}_Z(z) = N(z - \mu | 0, (I - B)^{-1} K) = N(z | \mu, (I - B)^{-1} K)$$

□

*Note 32.* When CAR is used for modeling,  $B$  is often specified to be sparse either due to some natural problem specific property, or for our computational convenience as it may allow the use of sparse solvers. To achieve this, one way is to specify  $B = \phi N$  where  $\phi > 0$  and  $N$  is an adjacency matrix; that is  $[B]_{i,j} = \phi 1(i \sim j) 1(i \neq j)$  will be non-zero only for adjacent pairs  $i$  and  $j$ .

*Note 33.* The system in (3.2) can be rewritten as

$$(3.4) \quad Z = \mu + B(Z - \mu) + E \iff E = (I - B)(Z - \mu)$$

by setting  $E = (I - B)(Z - \mu)$ . The distribution of  $Z$  in (3.2) induces a distribution on  $E$  as  $E \sim N(0, K(I - B)^\top)$  because

$$E(E) = E((I - B)(Z - \mu)) = (I - B)E(Z - \mu) = 0$$

$$\text{Var}(E) = \text{Var}((I - B)Z) = (I - B)\text{Var}(Z)(I - B)^\top = (I - B)(I - B)^{-1}K(I - B)^\top$$

### 3.2. Simultaneous Autoregressive (SAR) models.

*Note 34.* CAR sets the AR relation, and specifies the distribution on  $Z$  which induces the distribution on  $E$ ; see (3.4). SAR does the reverse; sets the same AR relation but it specifies the distribution on  $E$  which induces the distribution on  $Z$ —this is more might be more intuitive (?).

**Definition 35.** Consider discrete set of sites  $\mathcal{S} = \{s_i; i = 1, \dots, n\}$ . Consider a random field  $Z = (Z_s; s \in \mathcal{S})^\top = (Z_i = Z(s_i); i = 1, \dots, n)^\top$  on the discrete set of indexes  $\mathcal{S}$  with values in  $\mathcal{Z}$ . Define

$$Z = \mu + \tilde{B}(Z - \mu) + E \iff E = (I - \tilde{B})(Z - \mu)$$

Assume that matrix  $\tilde{B}$  is such that  $(I - \tilde{B})^{-1}$  exists, and  $[\tilde{B}]_{i,i} = 0$ . Assume that  $E = (E_i; i = 1, \dots, n)$  is an  $n$ -dimensional Gaussian random vector  $E \sim N_n(0, \Lambda)$  with  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$  whose elements are indexed by  $\mathcal{S}$ . Then we say that  $Z$  follows a “Gaussian” Simultaneous Autoregressive, SAR, model.

**Proposition 36.** The joint distribution of  $Z$  following the SAR model in Definition 35 is

$$(3.5) \quad Z \sim N\left(\mu, (I - \tilde{B})^{-1} \Lambda (I - \tilde{B}^\top)^{-1}\right)$$

*Proof.*  $Z$  is a linear combination of Gaussian random vecors, hence it follows a Gaussian distribution. Its mean and variance are

$$\begin{aligned} \mathbb{E}(Z) &= \mathbb{E}\left(\left(I - \tilde{B}\right)^{-1} E + \mu\right) = \mu, \\ \text{Var}(Z) &= \text{Var}\left(\left(I - \tilde{B}\right)^{-1} E + \mu\right) = \left(I - \tilde{B}\right)^{-1} \text{Var}(E) \left(I - \tilde{B}^\top\right)^{-1} = \left(I - \tilde{B}\right)^{-1} \Lambda \left(I - \tilde{B}^\top\right)^{-1} \end{aligned}$$

□

### 3.3. A comparison between CAR and SAR.

*Note 37.* We compare the use and flexibility of the two models.

*Remark 38.* From (3.2) and (3.5), CAR and SAR are equivalent iff

$$\underbrace{(I - B)^{-1} K}_{\text{CAR}} = \underbrace{\left(I - \tilde{B}\right)^{-1} \Lambda \left(I - \tilde{B}^\top\right)^{-1}}_{\text{SAR}}$$

*Note 39.* Following, we show that any SAR model can be written as a CAR model, however the converse is not always true.

**Proposition 40.** *Any positive-definite covariance matrix  $\Sigma$  can be expressed as the covariance matrix of a CAR model  $\Sigma_{\text{CAR}} = (I - B)^{-1} K$ , for a unique pair of matrices  $B$  and  $K$  where  $(I - B)$  is non-singular and  $K$  is diagonal.*

*Proof.* (This proof can be considered as an exercise for understanding CAR) Express

$$\Sigma^{-1} = D - R$$

for

$$[D]_{i,j} = \begin{cases} [\Sigma^{-1}]_{i,i} & i = j \\ 0 & i \neq j \end{cases}, \text{ and } [R]_{i,j} = \begin{cases} 0 & i = j \\ -[\Sigma^{-1}]_{i,j} & i \neq j \end{cases}$$

then

$$\Sigma = (D - R)^{-1} = (D(I - D^{-1}R))^{-1} = (I - D^{-1}R)^{-1} D^{-1}$$

Now define  $B = D^{-1}R$  and  $K = D^{-1}$ , and you get  $\Sigma = \Sigma_{\text{CAR}}$ . Now regarding the uniqueness, assume there is another pair of  $\mathring{B}$ , and  $\mathring{K}$  such that  $\Sigma_{\text{CAR}} = (I - \mathring{B})^{-1} \mathring{K}$ . Then

$$\text{diag}(\Sigma^{-1}) = \text{diag}(\Sigma_{\text{CAR}}^{-1}) = \text{diag}\left(\mathring{K}^{-1} (I - \mathring{B})\right) = \text{diag}\left(\mathring{K}^{-1}\right)$$

and similarly  $\text{diag}(\Sigma^{-1}) = \text{diag}(K^{-1})$ . Hence it has to be  $\mathring{K} = K$  because both are diagonal matrices. Then it is

$$(I - \mathring{B})^{-1} \mathring{K} = (I - B)^{-1} K \xLeftrightarrow{\mathring{K}=K} \mathring{B} = B.$$

So the representation is unique. □



**Proposition 41.** Any positive-definite covariance matrix  $\Sigma$  can be expressed as the covariance matrix of a SAR model  $\Sigma_{\text{SAR}} = (I - \tilde{B})^{-1} \Lambda (I - \tilde{B}^\top)^{-1}$  for a (non-unique) pair of matrices  $\tilde{B}$  and  $\Lambda$  where  $(I - \tilde{B})$  is non-singular,  $[\tilde{B}]_{i,i} = 0$ , and  $\Lambda$  is diagonal.

*Proof.* (This proof can be considered as an exercise for understanding SAR) Express

$$\Sigma^{-1} = LL^\top$$

where  $L$  is a lower triangular matrix with  $[L]_{i,i} > 0$ . Such matrix decomposition can be done by Cholesky decomposition, square-matrix decomposition, etc... and hence it is not always unique. Then

$$\Sigma = (LL^\top)^{-1} = L^{-\top} L^{-1}$$

Now express,  $L = D - C$  for

$$[D]_{i,j} = \begin{cases} [L]_{i,i} & i = j \\ 0 & i \neq j \end{cases}, \text{ and } [C]_{i,j} = \begin{cases} 0 & i = j \\ -[L]_{i,j} & i \neq j \end{cases}$$

then

$$\begin{aligned} \Sigma &= (D - C)^{-\top} (D - C)^{-1} = (I - D^{-1}C)^{-\top} D^{-\top} D^{-1} (I - D^{-1}C)^{-1} \\ &= (I - C^\top D^{-\top})^{-1} D^{-\top} D^{-1} (I - (C^\top D^{-\top})^\top)^{-1} \end{aligned}$$

Set  $\tilde{B} = C^\top D^{-\top}$  and  $\Lambda = D^{-\top} D^{-1}$  and you get  $\Sigma_{\text{SAR}} = \Sigma$  for non-unique pairs of  $\tilde{B}$  and  $\Lambda$ .  $\square$

**Proposition 42.** Any SAR model can be written as a unique CAR model.

*Proof.* (This proof can be considered as an exercise for understanding CAR/sar) SAR and CAR are both Gaussian's with the same mean. SAR's variance matrix is positive definite, and hence it can be written in a unique manner as a CAR's variance matrix by Proposition 40.  $\square$

**Proposition 43.** Any CAR model can be written as a non-unique SAR model.

*Proof.* SAR and CAR are both Gaussian's with the same mean. CAR's variance matrix is positive definite, and hence it can be written in a non-unique manner as a SAR's variance matrix by Proposition 41.  $\square$

**Example 44.** Show that

- (1)  $Z_i$  and  $E_j$  are independent for  $i \neq j$  in Gaussian CAR
- (2)  $Z_i$  and  $E_j$  are not necessarily independent for  $i \neq j$  in Gaussian SAR

**Solution.**

(1) For Gaussian CAR,

$$\text{Cov}(E, Z) = \text{Cov}((I - B)Z, Z) = (I - B)\text{Var}(Z) = (I - B)(I - B)^{-1}K = K$$

which is a diagonal; hence  $Z_i$  and  $E_j$  are independent for  $i \neq j$ .

(2) For Gaussian SAR,

$$\text{Cov}(Z, E) = \text{Cov}\left(\left(I - \tilde{B}\right)^{-1}E, E\right) = \left(I - \tilde{B}\right)^{-1}\text{Var}(E) = \left(I - \tilde{B}\right)^{-1}\Lambda$$

which is not a diagonal matrix in general; hence  $Z_i$  and  $E_j$  may be dependent for  $i \neq j$ .

#### 4. RELATED RANDOM FIELDS WITH PARTICULAR PROPERTIES

*Note 45.* We introduce more general modeling structures for basic spatial models which are computationally convenient yet quite descriptive for spatial statistical modeling. Convenient because they aim to break a high-dimensional problem into smaller ones using conditional independence, and reasonable because they allow representation of spatial dependence as well. We introduce the Gibbs Random Fields and the Markov Random Fields. The aforesaid Ising, CAR, and SAR models are just special cases of modeling structures.

##### 4.1. Gibbs Random Fields.

*Notation 46.* Recall notation  $z_{\mathcal{A}} = (z_i : i \in \mathcal{A})$  and  $\mathcal{Z}^{\mathcal{A}} = \{z_{\mathcal{A}} : z \in \mathcal{Z}^{\mathcal{S}}\}$  for  $\mathcal{A} \subseteq \mathcal{S}$ .

**Definition 47.** Let  $\mathcal{S} \neq \emptyset$  be a finite collection of sites. Let  $\mathcal{Z} \subset \mathbb{R}$ . Interaction potential is a family  $\mathcal{V} = \{V_{\mathcal{A}} : \mathcal{A} \subseteq \mathcal{S}\}$  of potential functions  $V_{\mathcal{A}} : \mathcal{Z}^{\mathcal{A}} \rightarrow \mathbb{R}$  such that  $V_{\emptyset}(\cdot) := 0$  and for every set  $\mathcal{A} \subseteq \mathcal{S}$  the sum

$$(4.1) \quad U_{\mathcal{A}}^{\mathcal{V}}(z) = \sum_{\{\mathcal{B} \subseteq \mathcal{S} : \mathcal{A} \cap \mathcal{B} \neq \emptyset\}} V_{\mathcal{B}}(z_{\mathcal{B}})$$

exists.

**Definition 48.** In Definition 47, the function  $V_{\mathcal{A}} : \mathcal{Z}^{\mathcal{A}} \rightarrow \mathbb{R}$  is called potential on  $\mathcal{A}$ .

**Definition 49.** In Definition 47, the function  $U_{\mathcal{A}}^{\mathcal{V}}(z)$  in (4.1) is called energy function of interaction potential  $\mathcal{V}$  on  $\mathcal{A}$  is called.

**Definition 50.** The interaction potential  $\mathcal{V}$  is said to be admissible if for all  $\mathcal{B} \subseteq \mathcal{S}$  and  $z_{\mathcal{S} \setminus \mathcal{B}} \in \mathcal{Z}^{\mathcal{S} \setminus \mathcal{B}}$

$$C_{\mathcal{A}}^{\mathcal{V}}(z_{\mathcal{S} \setminus \mathcal{A}}) = \int \exp(U_{\mathcal{A}}^{\mathcal{V}}((z_{\mathcal{A}}, z_{\mathcal{S} \setminus \mathcal{A}}))) dz_{\mathcal{A}} < \infty$$

*Note 51.* This allow as to define a distribution corresponding to the energy.

**Definition 52.** Let  $Z$  be  $\mathcal{Z}$  valued Random Field on a finite collection of sites  $\mathcal{S}$  with  $\mathcal{S} \neq \emptyset$ , and let  $\mathcal{V} = \{V_{\mathcal{A}} : \mathcal{A} \subseteq \mathcal{S}\}$  be an interaction potential of functions  $V_{\mathcal{A}} : \mathcal{Z}^{\mathcal{A}} \rightarrow \mathbb{R}$ . Assume that  $\mathcal{V}$  is admissible. Then  $Z$  is a Gibbs Random Field with interaction potentials  $\mathcal{V} = \{V_{\mathcal{A}} : \mathcal{A} \subseteq \mathcal{S}\}$  if

$$(4.2) \quad \text{pr}_Z(z_{\mathcal{A}} | z_{\mathcal{S} \setminus \mathcal{A}}) = \frac{1}{C_{\mathcal{A}}^{\mathcal{V}}(z_{\mathcal{S} \setminus \mathcal{A}})} \exp \left( \underbrace{\sum_{\{\mathcal{B} \subseteq \mathcal{S} : \mathcal{A} \cap \mathcal{B} \neq \emptyset\}} V_{\mathcal{B}}(z_{\mathcal{B}})}_{=U_{\mathcal{A}}^{\mathcal{V}}(z)} \right), \quad z \in \mathcal{Z}^{\mathcal{S}}$$

**Definition 53.** The normalizing integral  $C_{\mathcal{A}}^{\mathcal{V}}$  in (4.2) is called partition function.

*Notation 54.* For the marginal  $\text{pr}_Z(z_{\mathcal{S}})$  we will denote

$$\text{pr}_Z(z_{\mathcal{S}}) = \frac{1}{C_{\mathcal{S}}^{\mathcal{V}}} \exp(U_{\mathcal{S}}^{\mathcal{V}}(z)) = \frac{1}{C_{\mathcal{S}}^{\mathcal{V}}} \exp \left( \sum_{\mathcal{B} \subseteq \mathcal{S}} V_{\mathcal{B}}(z_{\mathcal{B}}) \right), \quad z \in \mathcal{Z}^{\mathcal{S}}$$

where  $C_{\mathcal{S}}^{\mathcal{V}} < \infty$  is the constant. In this case (and when it is clear), to easy the notation, we can omit  $\cdot_{\mathcal{S}}^{\mathcal{V}}$  and just write

$$\text{pr}_Z(z_{\mathcal{S}}) = \frac{1}{C} \exp \left( \sum_{\mathcal{B} \subseteq \mathcal{S}} V_{\mathcal{B}}(z_{\mathcal{B}}) \right), \quad z \in \mathcal{Z}^{\mathcal{S}}$$

**Example 55.** (Ising model) In Example 12, the Ising model (1.1) has potentials

$$\begin{aligned} V_{\emptyset}(z) &= 0 \\ V_{\{i\}}(z) &= \alpha z_i \quad \forall i \in \mathcal{S} \\ V_{\{i,j\}}(z) &= \begin{cases} \beta z_i z_j & \text{if } i \sim j \\ 0 & \text{if } i \not\sim j \end{cases} \\ V_{\mathcal{A}}(z) &= 0, \text{ if } \text{card}(\mathcal{A}) > 2 \end{aligned}$$

it has energy function

$$U(z) := U_{\mathcal{S}}^{\mathcal{V}}(z_{\mathcal{S}}) = \alpha \sum_{i \in \mathcal{S}} z_i + \beta \sum_{\{i \in \mathcal{S}, j \in \mathcal{S} : i \sim j\}} z_i z_j$$

and it has energy function conditional on  $\mathcal{S} \setminus \mathcal{B}$

$$U_{\mathcal{B}}^{\mathcal{V}}(z_{\mathcal{B}} | z_{\mathcal{S} \setminus \mathcal{B}}) = \alpha \sum_{i \in \mathcal{B}} z_i + \beta \sum_{\{i \in \mathcal{B}, j \in \mathcal{S} : i \sim j\}} z_i z_j$$

*Note 56.* In what follows we discuss identifiability matters related to the potential.

**Definition 57.** The interaction potential  $\mathcal{V}$  is said to be normalized with respect to a normalizing reference point  $\zeta \in \mathcal{Z}$  if there is  $i \in \mathcal{S}$  which for any  $z \in \mathcal{Z}^{\mathcal{S}}$  with  $z_i = \zeta$  implies that  $V_{\mathcal{B}}(z) = 0$ .

*Note 58.* In (4.2), the mapping  $\mathcal{V} \rightarrow \text{pr}_Z$  is in general non-identifiable because (4.2) can be constructed from a different interaction potential  $\tilde{\mathcal{V}} = \{V_{\mathcal{B}} + c : \mathcal{B} \subseteq \mathcal{S}\}$  for any constant  $c$ . I.e.  $U_{\mathcal{S}}^{\mathcal{V}}(z) = U_{\mathcal{S}}^{\tilde{\mathcal{V}}}(z)$ .

*Note 59.* One way to make  $\mathcal{V}$  identifiable is to impose restriction

$$(4.3) \quad \forall \mathcal{A} \neq \emptyset, V_{\mathcal{A}}(z) = 0, \text{ if for some } i \in \mathcal{A}, z_i = \zeta$$

*Notation 60.* For convenience, consider notation related to  $z^{[\mathcal{B}, \zeta]}$  such as

$$[z^{[\mathcal{B}, \zeta]}]_i = \begin{cases} \zeta, & \text{if } i \notin \mathcal{B} \\ z_i, & \text{if } i \in \mathcal{B} \end{cases}$$

and  $z_{\mathcal{A}}^{[\mathcal{B}, \zeta]} = (z_s^{[\mathcal{B}, \zeta]}; s \in \mathcal{A})$ , and  $z_s^{[\mathcal{B}, \zeta]} = z_{\{s\}}^{[\mathcal{B}, \zeta]}$  for some fixed  $\zeta$ .

**Example 61.** For instance if  $z \in \mathcal{Z}^{\mathcal{S}}$  where  $\mathcal{S} = \{1, \dots, n\}$  then

$$\begin{aligned} z^{[\emptyset, \zeta]} &= \left( \overbrace{\zeta, \dots, \zeta}^{n \text{ times}} \right)^{\top}; & z^{[\{i\}, \zeta]} &= \left( \zeta, \dots, \zeta, \overbrace{z_i}^{i\text{th location}}, \zeta, \dots, \zeta \right)^{\top}; \\ z^{[\{i, j\}, \zeta]} &= \left( \zeta, \dots, \zeta, \overbrace{z_i}^{i\text{th location}}, \zeta, \dots, \zeta, \overbrace{z_j}^{j\text{th location}}, \dots, \zeta \right)^{\top}; & z^{[\mathcal{S}, \zeta]} &= (z_1, \dots, z_n)^{\top}; \end{aligned}$$

*Note 62.* The following theorem uniquely associates potentials satisfying (4.3) with (4.2) with regards a normalizing point.

**Theorem 63.** Let  $Z$  be an  $\mathcal{Z}$ -valued random field on a finite collection  $\mathcal{S} \neq \emptyset$  of sites such that  $\text{pr}_Z(z) > 0$  for all  $z \in \mathcal{Z}^{\mathcal{S}}$ . Then  $Z$  is a Gibbs Random Field with respect to the canonical potential

$$\begin{aligned} (4.4) \quad V_{\mathcal{A}}(z_{\mathcal{A}}) &= \sum_{\mathcal{B} \subseteq \mathcal{A}} (-1)^{\text{Card}(\mathcal{A} \setminus \mathcal{B})} U_{\mathcal{B}}^{\mathcal{V}}(z^{[\mathcal{B}, \zeta]}), \quad z \in \mathcal{Z}^{\mathcal{S}} \\ &= \sum_{\mathcal{B} \subseteq \mathcal{A}} (-1)^{\text{Card}(\mathcal{A} \setminus \mathcal{B})} \log(\text{pr}_Z(z^{[\mathcal{B}, \zeta]})), \quad z \in \mathcal{Z}^{\mathcal{S}} \end{aligned}$$

where  $\zeta \in \mathcal{Z}$  is a fixed value and notation  $z^{[\mathcal{B}, \zeta]}$  denotes the vector based on  $z \in \mathcal{Z}^{\mathcal{S}}$  but modified such that its  $i$ -th element is  $[z^{[\mathcal{B}, \zeta]}]_i = z_i$  if  $i \in \mathcal{B}$  and  $[z^{[\mathcal{B}, \zeta]}]_i = \zeta$  if  $i \notin \mathcal{B}$ . This is the unique normalized potential w.r.t  $\zeta \in \mathcal{Z}$ .

*Proof.* The proof is based on Möbius inversion formula, and hence out of scope.  $\square$

**Corollary 64.** *From Theorem 63, for all  $i \in \mathcal{A}$  it is*

$$(4.5) \quad V_{\mathcal{A}}(z_{\mathcal{A}}) = \sum_{\mathcal{B} \subseteq \mathcal{A}} (-1)^{\text{Card}(\mathcal{A} \setminus \mathcal{B})} \log \left( pr_i \left( z_i^{[\mathcal{B}, \zeta]} | z_{\mathcal{S} \setminus \{i\}}^{[\mathcal{B}, \zeta]} \right) \right), \quad z \in \mathcal{Z}^{\mathcal{S}}$$

*Note 65.* The following example explains the use of Theorem 63 in terms of the Definition 47.

**Example 66.** Consider  $\mathcal{S} = \{1, 2\}$ . Let  $z = (z_1, z_2)^{\top}$ . Consider a fixed  $\zeta \in \mathcal{Z}$ . Then  $\mathcal{V} = \{V_{\mathcal{A}} : \mathcal{A} \subseteq \mathcal{S}\} = \{V_{\{1\}}, V_{\{2\}}, V_{\{1,2\}}\}$ . The decomposition of the energy  $U(z = (z_1, z_2)^{\top}) := U_{\mathcal{S}}^{\mathcal{V}}(z)$  is written as

$$U(z_1, z_2) - U(\zeta, \zeta) = V_{\{1\}}(z_1) + V_{\{2\}}(z_2) + V_{\{1,2\}}(z_1, z_2)$$

by using (4.1) with

$$V_{\{1\}}(z_1) = U(z_1, \zeta) - U(\zeta, \zeta)$$

$$V_{\{2\}}(z_2) = U(\zeta, z_2) - U(\zeta, \zeta)$$

$$V_{\{1,2\}}(z_1, z_2) = U(z_1, z_2) - U(z_1, \zeta) - U(\zeta, z_2) + U(\zeta, \zeta)$$

by (4.4).

**Example 67.** (Ising model) We revisit Example 12 where

$$\text{pr}_{\mathcal{Z}}(z) \propto \exp \left( \alpha \sum_{i \in \mathcal{S}} z_i + \beta \sum_{\{i,j\}: i \sim j} z_i z_j \right), \quad \forall z \in \mathcal{Z}^{\mathcal{S}}$$

Consider Notation 60, for instance,

$$\begin{aligned} z^{[\emptyset, \zeta]} &= \left( \overbrace{\zeta, \dots, \zeta}^{n \text{ times}} \right)^{\top}; & z^{[\{i\}, \zeta]} &= \left( \zeta, \dots, \zeta, \underbrace{\zeta_i}_{\substack{\downarrow \\ \text{i-th location}}}, \zeta, \dots, \zeta \right)^{\top}; \\ z^{[\{i,j\}, \zeta]} &= \left( \zeta, \dots, \zeta, \underbrace{\zeta_i}_{\substack{\downarrow \\ \text{i-th location}}}, \zeta, \dots, \zeta, \underbrace{\zeta_j}_{\substack{\downarrow \\ \text{j-th location}}}, \dots, \zeta \right)^{\top}; & z^{[\mathcal{S}, \zeta]} &= (z_1, \dots, z_n)^{\top}; \end{aligned}$$

It is  $V_{\emptyset} = 0$  by definition. By using Theorem 63 and considering a reference point  $\zeta = 0$ , we get

$$(4.6) \quad V_{\{i\}}(z) = (-1)^{1-1} U(z^{[\{i\}, \zeta]}) + (-1)^{1-0} U(z^{[\emptyset, \zeta]}) = az_i,$$

for any  $i \in \mathcal{S}$  and

$$\begin{aligned}
 (4.7) \quad V_{\{i,j\}}(z) &= [(-1)^{2-2} U(z^{\{\{i,j\}, \zeta\}})] + [(-1)^{2-1} U(z^{\{\{i\}, \zeta\}})] \\
 &\quad + [(-1)^{2-1} U(z^{\{\{j\}, \zeta\}})] + [(-1)^{2-0} U(z^{\{\emptyset, \zeta\}})] \\
 &= [\alpha z_i + \alpha z_j + \beta z_i z_j] + [-\alpha z_i] + [-\alpha z_j] + [0] = \beta z_i z_j
 \end{aligned}$$

for any  $i, j \in \mathcal{S}$ , with  $i \sim j$ . Obviously, it is  $V_{\{i,j\}}(z) = 0$  for any  $i, j \in \mathcal{S}$ , with  $i \not\sim j$ ; and it is  $V_{\mathcal{A}}(z) = 0$  for  $\text{card}(\mathcal{A}) > 2$ .

## 4.2. Markov Random Fields.

*Note 68.* Regarding spatial modeling,  $\sim$  can describe adjacent sites which is in accordance to the spatial statistics “dogma” that *near things are more related than distant things*. Also it may be computationally convenient for big data problems (large number of sites) as it introduces sparsity and allows specialized numerical algorithms to be implemented.

*Note 69.* Markov Random Fields constrain the problem such that the conditional distribution of the label at some site  $i$  given those at all other sites  $j \in \mathcal{S} - \{i\}$  depends only on the labels at neighbors of site  $i$ .

**Example 70.** Recall the Ising model in Example 67 whose sites are equipped with a symmetric relation “ $\sim$ ”. Its potentials  $V_{\mathcal{A}}$  are non-zero only when  $\mathcal{A}$  is a pair of sites  $\{i, j\}$  satisfying the relation  $\sim$  (4.7) or when  $\mathcal{A}$  a singleton (4.6). Consequently, its local characteristics  $\text{pr}_i(z_i | z_{\mathcal{S} \setminus \{i\}})$  depend only on the values of the sites  $j \in \mathcal{S} \setminus \{i\}$  that satisfy  $\sim$ .

**Definition 71.** We define as the boundary of  $\mathcal{A}$ ,  $\mathcal{A} \subseteq \mathcal{S}$ , for a given relation  $\sim$  the set

$$\partial \mathcal{A} = \{s \in \mathcal{S} \setminus \mathcal{A} : \exists t \in \mathcal{A} \text{ s.t. } s \sim t\}$$

**Definition 72.** Let  $\partial \mathcal{A}$  be the boundary of  $\mathcal{A} \subseteq \mathcal{S}$  for a symmetric relation  $\sim$  the finite set  $\mathcal{S} \neq \emptyset$ .  $Z$  is a random field on  $\mathcal{S}$  taking values in  $\mathcal{Z}$  with respect to the symmetric relation  $\sim$  if for each  $\mathcal{A} \subset \mathcal{S}$  and  $Z_{\mathcal{A} \setminus \mathcal{S}} \in \mathcal{Z}_{\mathcal{A} \setminus \mathcal{S}}$  the distribution of  $Z$  on  $\mathcal{A}$  conditional on  $Z_{\mathcal{A} \setminus \mathcal{S}}$  only depends on  $Z_{\partial \mathcal{A}}$  (i.e. the configuration of  $Z$  on the neighborhood boundary of  $\mathcal{A}$ ) i.e.

$$(4.8) \quad \text{pr}_Z(z_{\mathcal{A}} | z_{\mathcal{S} \setminus \mathcal{A}}) = \text{pr}_Z(z_{\mathcal{A}} | z_{\partial \mathcal{A}})$$

when  $\text{pr}_Z(z_{\mathcal{S} \setminus \mathcal{A}}) > 0$

*Note 73.* Definition 72 implies that (4.8) becomes

$$(4.9) \quad \text{pr}_Z(z_i | z_{-i}) = \text{pr}_Z(z_i | z_{\partial \{i\}}), \quad \forall i \in \mathcal{S}$$

when  $\text{pr}_Z(z_{\mathcal{S} \setminus \{i\}}) > 0$

**Definition 74.** A non-empty subset  $\mathcal{C}$ ,  $\mathcal{C} \subset \mathcal{S}$ , is a clique in  $\mathcal{S}$  with respect to  $\sim$  if for all  $s, t \in \mathcal{C}$  with  $s \neq t$  it is  $s \sim t$  or if  $\mathcal{C}$  is a singleton set.

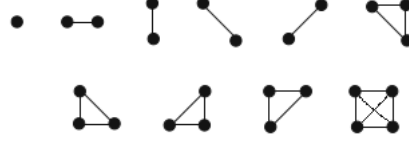


FIGURE 4.1. Examples of cliques

*Notation 75.* The set containing all the cliques in a lattice of sites in  $\mathcal{S}$  equipped with a relation  $\sim$  will be usually denoted as bold  $\mathcal{C}$ .

*Note 76.* The following theorem shows that the distribution of any Markov random field such that  $pr_Z(z) > 0$  can be expressed in terms of interactions between neighbors.

**Theorem 77.** (*Hammersley–Clifford*) Let  $Z$  be an  $\mathcal{Z}$ -valued random field on a finite collection  $\mathcal{S} \neq \emptyset$  of sites such that  $pr_Z(z_{\mathcal{A}}|z_{\mathcal{C} \setminus \mathcal{A}}) > 0$  for all  $\mathcal{A} \subset \mathcal{S}$  and  $z \in \mathcal{Z}^{\mathcal{S}}$ . Let  $\sim$  be a symmetric relation on  $\mathcal{S}$ . Then  $Z$  is a Markov Random Field with respect to  $\sim$  if and only if

$$(4.10) \quad pr_Z(z) \propto \prod_{\mathcal{C} \in \mathcal{C}} \varphi_{\mathcal{C}}(z_{\mathcal{C}})$$

for some interaction functions  $\varphi_{\mathcal{C}} : \mathcal{Z}^{\mathcal{C}} \rightarrow \mathbb{R}^+$  defined on cliques  $\mathcal{C} \in \mathcal{C}$ .

*Proof.* □

For convenience, let  $[z^{\mathcal{B}, \delta}]_i = \begin{cases} \delta, & \text{if } i \notin \mathcal{B} \\ z_i, & \text{if } i \in \mathcal{B} \end{cases}$ , and  $z_{\mathcal{A}}^{\mathcal{B}, \delta} = (z_s^{\mathcal{B}, \delta}; s \in \mathcal{A})$ , and  $z_s^{\mathcal{B}, \delta} = z_{\{s\}}^{\mathcal{B}, \delta}$ .

**for  $\implies$ :** By Theorem 63,  $Z$  is Gibbs with a canonical potential (4.4)

$$V_{\mathcal{A}}(z_{\mathcal{A}}) = \sum_{\mathcal{A} \subseteq \mathcal{B}} (-1)^{\text{Card}(\mathcal{A} \setminus \mathcal{B})} \log(pr_Z(z^{\mathcal{B}, \mathcal{A}})),$$

for  $z \in \mathcal{Z}^{\mathcal{S}}$ . We need to show that for all  $\mathcal{A}$  which are not a cliques,  $\mathcal{A} \notin \mathcal{C}$ .

Assume a set  $\mathcal{A}$  with  $\mathcal{A} \subseteq \mathcal{S}$  which is not a clique,  $\mathcal{A} \notin \mathcal{C}$ , there are two distinct sites  $s, t \in \mathcal{A}$  with  $s \not\sim t$ . Then,

$$\begin{aligned}
V_{\mathcal{A}}(z) &= \sum_{\mathcal{B} \subseteq \mathcal{A}} (-1)^{\text{Card}(\mathcal{A} \setminus \mathcal{B})} \log \left( pr_Z \left( z_s^{\mathcal{B}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B}, \delta} \right) \right) \\
&= \sum_{\mathcal{B} \subseteq \mathcal{A} \setminus \{s, t\}} (-1)^{\text{Card}(\mathcal{A} \setminus \mathcal{B})} \log \left( pr_Z \left( z_s^{\mathcal{B}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B}, \delta} \right) \right) \\
&\quad + \sum_{\mathcal{B} \subseteq \mathcal{A} \setminus \{s, t\}} (-1)^{\text{Card}(\mathcal{A} \setminus (\mathcal{B} \cup \{s\}))} \log \left( pr_Z \left( z_s^{\mathcal{B} \cup \{s\}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B} \cup \{s\}, \delta} \right) \right) \\
&\quad + \sum_{\mathcal{B} \subseteq \mathcal{A} \setminus \{s, t\}} (-1)^{\text{Card}(\mathcal{A} \setminus (\mathcal{B} \cup \{t\}))} \log \left( pr_Z \left( z_s^{\mathcal{B} \cup \{t\}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B} \cup \{t\}, \delta} \right) \right) \\
&\quad + \sum_{\mathcal{B} \subseteq \mathcal{A} \setminus \{s, t\}} (-1)^{\text{Card}(\mathcal{A} \setminus (\mathcal{B} \cup \{s, t\}))} \log \left( pr_Z \left( z_s^{\mathcal{B} \cup \{s, t\}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B} \cup \{s, t\}, \delta} \right) \right)
\end{aligned}$$

Rearranging I get simplifies

$$V_{\mathcal{A}}(z) = \sum_{\mathcal{B} \subseteq \mathcal{A}} (-1)^{\text{Card}(\mathcal{A} \setminus \mathcal{B})} \log \left( \frac{pr_Z \left( z_s^{\mathcal{B}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B}, \delta} \right)}{pr_Z \left( z_s^{\mathcal{B} \cup \{t\}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B} \cup \{t\}, \delta} \right)} \frac{pr_Z \left( z_s^{\mathcal{B} \cup \{s, t\}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B} \cup \{s, t\}, \delta} \right)}{pr_Z \left( z_s^{\mathcal{B} \cup \{s\}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B} \cup \{s\}, \delta} \right)} \right)$$

Because  $s \not\sim t$ , it is  $pr_Z \left( z_s^{\mathcal{B}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B}, \delta} \right) = pr_Z \left( z_s^{\mathcal{B} \cup \{t\}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B} \cup \{t\}, \delta} \right)$  and  $pr_Z \left( z_s^{\mathcal{B} \cup \{s, t\}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B} \cup \{s, t\}, \delta} \right) = pr_Z \left( z_s^{\mathcal{B} \cup \{s\}, \delta} | z_{\mathcal{S} \setminus s}^{\mathcal{B} \cup \{s\}, \delta} \right)$ . This implies  $V_{\mathcal{A}}(z) = 0$  for any subset  $\mathcal{A}$  with  $\mathcal{A} \subseteq \mathcal{S}$  which is not a clique. Hence (4.10) holds.

**for  $\Leftarrow$ :** By using (4.2), I can write

$$pr_Z(z_{\mathcal{A}} | z_{\mathcal{S} \setminus \mathcal{A}}) = \frac{1}{C_{\mathcal{A}}(z_{\mathcal{S} \setminus \mathcal{A}})} \exp(U_{\mathcal{A}}(z))$$

where

$$U_{\mathcal{A}}(z) = \sum_{\{C \subseteq \mathcal{S} : \mathcal{A} \cap C \neq \emptyset\}} V_C(z_C)$$

depends only on  $\{z_i : i \in \mathcal{A} \cup \partial \mathcal{A}\}$  as  $pr_Z(\cdot)$  is a Markov Random Field.

*Note 78.* Because  $pr_Z(z) > 0$ , the Markov Random Field in (4.10) is a Gibbs Random Field as

$$pr_Z(z) \propto \exp \left( \sum_{C \in \mathcal{C}} \log(\varphi_C(z_C)) \right)$$

with non-zero interaction potentials restricted to cliques  $C \in \mathcal{C}$ .

*Note 79.* Essentially Theorem 77 gives guidelines on using Markov RF and Gibbs RF that:



**for  $\implies$ :** we need to show that there exists an interaction potential  $\varphi = \{\varphi_{\mathcal{C}} : \mathcal{C} \in \mathcal{C}\}$  defined on the cliques  $\mathcal{C}$  such that  $\text{pr}_Z(\cdot)$  is a Gibbs Random Field with interaction potential  $\varphi$ .

**for  $\impliedby$ :** a Gibbs Random Field with potentials  $\{\varphi_{\mathcal{C}} : \mathcal{C} \in \mathcal{C}\}$  defined on the cliques  $\mathcal{C}$  is a Markov Random Field.

**Example 80.** (Ising model; Cont. Example 12). The joint PMF of the Ising model in Example 12 is

$$\begin{aligned} \text{pr}(z) &= \frac{\exp\left(\alpha \sum_{i \in \mathcal{S}} z_i + \beta \sum_{\{i,j\}: i \sim j} z_i z_j\right)}{\sum_{z \in \mathcal{Z}^{\mathcal{S}}} \exp\left(\alpha \sum_{i \in \mathcal{S}} z_i + \beta \sum_{\{i,j\}: i \sim j} z_i z_j\right)} \\ &= \frac{1}{\sum_{z \in \mathcal{Z}^{\mathcal{S}}} \exp\left(\alpha \sum_{i \in \mathcal{S}} z_i + \beta \sum_{\{i,j\}: i \sim j} z_i z_j\right)} \prod_{i \in \mathcal{S}} \exp(\alpha z_i) \prod_{i \in \mathcal{S}} \prod_{j: j \sim i} \exp(\beta z_i z_j) \end{aligned}$$

I can find that

$$\varphi_{\emptyset} = 1 / \sum_{z \in \mathcal{Z}^{\mathcal{S}}} \exp\left(\alpha \sum_{i \in \mathcal{S}} z_i + \beta \sum_{\{i,j\}: i \sim j} z_i z_j\right)$$

$$(4.11) \quad \varphi_{\{i\}}(z_{\{i\}}) = \exp(\alpha z_i), \quad \forall i \in \mathcal{S}$$

$$(4.12) \quad \begin{aligned} \varphi_{\{i,j\}}(z_{\{i,j\}}) &= \exp(\beta z_i z_j), & \forall i, j \in \mathcal{S} \quad \text{s.t.} \quad i \sim j \\ \varphi_{\{i,j\}}(z_{\{i,j\}}) &= 1, & \forall i, j \in \mathcal{S} \quad \text{s.t.} \quad i \not\sim j \\ \varphi_{\mathcal{A}}(z_{\mathcal{A}}) &= 1, & \forall \mathcal{A} \subset \mathcal{S} \quad \text{s.t.} \quad \text{card}(\mathcal{A}) > 2 \end{aligned}$$

where  $\{i\}$  and  $\{i, j\}$  satisfying  $i \sim j$  are cliques. Alternatively, as  $\emptyset$  is not a clique if that  $\varphi_{\emptyset}$  is just the constant term which can be absorbed by (4.11) and (4.12) and correspond to cliques.

## Part 2. Model building for aerial data & related inference

### 5. AUTOMODELS

*Note 81.* We introduce a general class of models, the automodels and their special case Besag's automodels, which are associated to the exponential family of distributions and able to represent spatial dependence.

**Definition 82.** A random variable  $X$  taking values in  $\mathcal{X}$  follows an exponential family labeled by parameter  $\theta \in \Theta$  if the associated PMF/PDF  $\text{pr}_X(x|\theta)$  can be expressed in the form

$$\text{pr}_X(x|\theta) = \exp\left(A(\theta)^\top B(x) + C(x) + D(\theta)\right), \quad \forall x \in \mathcal{X}$$

where  $A(\cdot)$ ,  $B(\cdot)$ ,  $C(\cdot)$ , and  $D(\cdot)$  are known functions.

### 5.1. Multi-parameter automodels.

**Theorem 83.** *Consider Markov random field  $Z$  that takes values in  $\mathcal{Z}$  on a finite set of points  $\mathcal{S}$  and has marginal probability*

$$(5.1) \quad pr_Z(z) = \frac{\exp(U(z))}{\int \exp(U(z)) dz}, \quad z \in \mathcal{Z}^{\mathcal{S}}.$$

*Consider some fixed normalization configuration  $\zeta = (\zeta, \dots, \zeta)^\top \in \mathcal{Z}^{\mathcal{S}}$ . Assume that the following assumptions are satisfied:*

(1) *In the energy function  $U(\cdot)$  the dependence between the sites is pairwise only, i.e.*

$$U(z) = \sum_{i \in \mathcal{S}} V_i(z_i) + \sum_{\{\{i,j\} \in \mathcal{S}^2: i \sim j\}} V_{i,j}(z_i, z_j), \quad z \in \mathcal{Z}_{\mathcal{S}}$$

*with  $V_i(\zeta) = V_{i,j}(z_i, \zeta) = V_{i,j}(\zeta, z_j) = 0$  for all  $i, j \in \mathcal{S}$ .*

(2) *For all  $i \in \mathcal{S}$ , the conditional distributions (characteristics) are exponential family distributions*

$$(5.2) \quad \log(pr_i(z_i|z_{-i})) = (A_i(z_{-i}))^\top B_i(z_i) + C_i(z_i) + D_i(z_{-i}),$$

*where  $A_i(z_{-i}) \in \mathbb{R}^\ell$ ,  $B_i(z_i) \in \mathbb{R}^\ell$ , for  $\ell \geq 1$  and  $C_i(z_i) \in \mathbb{R}$ , and  $D_i(z_{-i}) \in \mathbb{R}$  with  $C_i(\zeta) = 0$  and  $D_i(\zeta, \dots, \zeta) = 0$ .*

(3) *For all  $i \in \mathcal{S}$ ,  $\text{span}\{B_i(z_i); z_i \in \mathcal{Z}\} = \mathbb{R}^\ell$ , for  $\ell \geq 1$ .*

*Then, necessarily,*

(1) *the functions  $A_i(z_{-i}) \in \mathbb{R}^\ell$  take the form*

$$A_i(z_{-i}) = \alpha_i + \sum_{i \neq j} \beta_{i,j} B_j(z_j), \quad i \in \mathcal{S}$$

*where  $\{\alpha_i; i \in \mathcal{S}\}$  is a family of  $\ell$ -dimensional vectors, and  $\{\beta_{i,j}; i, j \in \mathcal{S}, i \neq j\}$  is a family of  $\ell \times \ell$  symmetric matrices, and*

(2) *the potentials are given by*

$$(5.3) \quad V_i(z_i) = (\alpha_i)^\top B_i(z_i) + C_i(z_i)$$

$$(5.4) \quad V_{i,j}(z_i, z_j) = (B_i(z_i))^\top \beta_{i,j} B_j(z_j)$$

*Proof.* Omitted, but can be found in

- (1) Hardouin, C., & Yao, J. F. (2008). Multi-parameter automodels and their applications. *Biometrika*, 95(2), 335-349.
- (2) Besag, J. (1974). Spatial interaction and the statistical analysis of lattice systems. *Journal of the Royal Statistical Society: Series B (Methodological)*, 36(2), 192-225.

□

**Definition 84.** Automodel is called the model satisfying the assumptions of Theorem 83.

**Definition 85.** Univariate automodel is the automodel with  $\ell = 1$  in Theorem 83.

**Definition 86.** **Multi-parameter** automodel with  $\ell \geq 1$  in Theorem 83.

*Remark 87.* In the univariate automodel,  $\ell = 1$ , assumption 3 in Theorem 83 is not needed; it is automatically satisfied as  $B_i$ 's are not identically zero. Yet, for  $\ell = 1$ , (5.3) and (5.4) become

$$(5.5) \quad V_i(z_i) = \alpha_i B_i(z_i) + C_i(z_i)$$

$$(5.6) \quad V_{i,j}(z_i, z_j) = \beta_{i,j} B_i(z_i) B_j(z_j)$$

## 5.2. Besag auto-models.

**Definition.**  $Z$  follows a Besag's auto-model if  $Z$  is real-valued and its joint distribution  $\text{pr}_Z(z)$  is given by

$$(5.7) \quad \text{pr}_Z(z) = \frac{1}{C} \exp \left( \sum_{i \in \mathcal{S}} V_i(z_i) + \sum_{\{i,j\} \in \mathcal{S}^2: i \sim j} \beta_{i,j} z_i z_j \right), \quad z \in \mathcal{Z}_{\mathcal{S}}$$

with  $\beta_{i,j} = \beta_{j,i}$  for all  $i, j \in \mathcal{S}$ .

*Note 88.* The following allows us to define a Markov Random Field model from a set of conditional distributions (characteristics) whose compatibility is automatically satisfied.

**Proposition 89.** *If each of the*

$$\text{pr}_i(z_i | z_{-i}), \quad \text{for } i \in \mathcal{S}$$

*is a family of real-valued  $z_i \in \mathbb{R}$  conditional distributions which are members of the exponential family of distributions (5.2) with  $B_i(z_i) = z_i$  for  $i \in \mathcal{S}$ , then they are compatible a Besag's auto-model with distribution (5.7) if  $\beta_{i,j} = \beta_{j,i}$  for all  $i, j \in \mathcal{S}$ .*

*Proof.* For

$$\text{pr}_i(z_i | z_{-i}) = \exp(A_i(z_{-i}) z_i + C_i(z_i) + D_i(z_{-i}))$$

it is

$$\begin{aligned} V_i(z_i) &= \alpha_i B_i(z_i) + C_i(z_i) = \alpha_i z_i + C_i(z_i) \\ V_{i,j}(z_i, z_j) &= \beta_{i,j} B_i(z_i) B_j(z_j) = \beta_{i,j} z_i z_j \end{aligned}$$

so

$$\text{pr}_Z(z) \propto \exp \left( \sum_i [\alpha_i z_i + C_i(z_i)] + \sum_{i \sim j} \beta_{i,j} z_i z_j \right), \quad z \in \mathcal{Z}_{\mathcal{S}}$$

□

**Example 90.** (Logistic automodel / Ising model) Consider that  $Z(s)$  represents presence or absence of a characteristic at location  $s \in \mathcal{S}$ . Mathematically, assume random field  $Z$  taking values on a set of indices  $\mathcal{S}$  in  $\mathcal{Z} = \{0, 1\}$  on  $\mathcal{S} = \{1, \dots, n\}$ ,  $n \in \mathbb{N} - \{0\}$ .

Consider that for a given  $z_{-i}$  it is

$$z_i | z_{-i} \sim \text{Logistic}(\theta_i(z_{-i})), \quad i \in \mathcal{S}.$$

**Hint::** The PMF of Logistic distribution  $x|\theta \sim \text{Logistic}(\theta)$  can be written as  $\text{pr}(x|\theta) = (1 - \exp(x\theta))^{-1} 1(x \in \{0, 1\})$ .

Then the characteristics are

$$(5.8) \quad \text{pr}_i(z_i | z_{-i}) = \frac{\exp(z_i \theta_i(z_{-i}))}{1 + \exp(\theta_i(z_{-i}))} 1(z_i \in \{0, 1\})$$

Now, let's parameterize  $\{\theta_i(\cdot)\}$  as

$$(5.9) \quad \theta_i(z_{-i}) = \alpha_i + \sum_{j:j \sim i} \beta_{i,j} z_j$$

for  $\{\alpha_i\}$  and  $\{\beta_{i,j}\}$  with  $\beta_{i,j} = \beta_{j,i}$ . Then (5.8) becomes

$$(5.10) \quad \log(\text{pr}_i(z_i | z_{-i})) = \underbrace{\underbrace{z_i}_{B_i(z_i)} \left( \underbrace{\alpha_i + \sum_{j \sim i} \beta_{i,j} z_j}_{A_i(z_{-i})} \right)}_{A_i(z_{-i})} + \underbrace{0}_{C_i(z_i)} + \underbrace{\left( -\log \left( 1 + \exp \left( \alpha_i + \sum_{j:j \sim i} \beta_{i,j} z_j \right) \right) \right)}_{D_i(z_{-i})}$$

Notice that all the conditionals  $z_i | z_{-i}$  follow an Exponential family with

$$A_i(z_{-i}) = \alpha_i + \sum_{j \sim i} \beta_{i,j} B_i(z_j)$$

$$B_i(z_i) = z_i$$

$$C_i(z_i) = 0$$

$$D_i(z_{-i}) = -\log \left( 1 + \exp \left( \alpha_i + \sum_{j:j \sim i} \beta_{i,j} z_j \right) \right)$$

Also, I can get  $C_i(\zeta) = 0$  and  $D_i(\zeta, \dots, \zeta) = 0$  by considering a reference point  $\zeta = 0$ . From Theorem 89, (5.8) with (5.9), the conditionals  $z_i | z_{-i}$  are compatible as a Besag auto-model

with marginal distribution

$$(5.11) \quad \text{pr}_Z(z) \propto \exp \left( \overbrace{\sum_i \alpha_i z_i}^{U(z)=} + \underbrace{\sum_i \sum_{j:j \sim i} \beta_{i,j} z_i z_j}_{\sum_{\{i,j\}:j \sim i} \underbrace{\beta_{i,j} z_i z_j}_{B_i(z_i)}} \right)$$

I observe that:

- Here the Ising model has spatially dependent coefficients  $\{\alpha_i\}$  and  $\{\beta_{i,j}\}$ , unlike the Ising model in Example 12 where we considered  $\{\alpha_i = \alpha\}$  and  $\{\beta_{i,j} = \beta\}$ .
- When  $\beta_{i,j} = 0$ , for all  $j$  such as  $j \sim i$ , it is  $\text{pr}_i(z_i | z_{-i}) = \frac{\exp(\alpha_i)}{1 + \exp(\alpha_i)}$ .
- Characteristic's present at site  $i$  is encouraged in neighboring site  $j$  when  $\beta_{i,j} > 0$ , and discouraged when  $\beta_{i,j} < 0$ .

The resulting spatial model is called Logistic automodel or Ising model (the latter name is from physics).

**Example 91.** ( Poisson automodel ) Consider that  $Z(s)$  represents counts at location  $s \in \mathcal{S}$ . Mathematically we can consider  $Z$  taking values in  $\mathcal{Z} = \mathbb{N}$  on a set of sites  $\mathcal{S} = \{1, \dots, n\}$ , where  $n \in \mathbb{N} - \{0\}$ .

Consider that for a given  $z_{-i}$  it is

$$z_i | z_{-i} \sim \text{Poisson}(\lambda_i(z_{-i}))$$

**Hint::** The PMF of Poisson distribution  $x | \lambda \sim \text{Poisson}(\lambda)$  can be written as

$$\text{pr}(x | \lambda) = \frac{1}{x!} \lambda^x \exp(-\lambda) \mathbf{1}(x \in \mathbb{N})$$

with mean  $E(x | \lambda) = \lambda$ .

Then the full conditionals (characteristics) are

$$(5.12) \quad \text{pr}_i(z_i | z_{-i}) = \frac{1}{z_i!} (\lambda_i(z_{-i}))^{z_i} \exp(-\lambda) \mathbf{1}(z_i \in \mathbb{N})$$

Now, let's parameterize  $\{\lambda_i(\cdot)\}$  as

$$(5.13) \quad \log(\lambda_i(z_{-i})) = \alpha_i + \sum_{j:j \sim i} \beta_{i,j} z_j$$

for  $\{\alpha_i\}$  and  $\{\beta_{i,j}\}$  with  $\beta_{i,j} = \beta_{j,i}$ . So (5.12) becomes

$$\log(\text{pr}_i(z_i | z_{-i})) = \underbrace{\underbrace{z_i}_{B_i(z_i)} \left( \underbrace{\alpha_i + \sum_{j \sim i} \beta_{i,j} \underbrace{z_j}_{B_i(z_j)}}_{A_i(z_{-i})} \right)}_{A_i(z_{-i})} + \underbrace{\log(z_i!)}_{C_i(z_i)} + \underbrace{0}_{D_i(z_{-i})}$$

with

$$\begin{aligned}
A_i(z_{-i}) &= z_i \\
B_i(z_i) &= \alpha_i + \sum_{j \sim i} \beta_{i,j} B_i(z_j) \\
C_i(z_i) &= \log(z_i!) \\
D_i(z_{-i}) &= 0
\end{aligned}$$

I can notice that all the conditionals  $z_i|z_{-i}$  follow exponential of exponential. Also, I can get  $C_i(\zeta) = 0$  and  $D_i(\zeta, \dots, \zeta) = 0$  by considering a reference point  $\zeta = 0$ . From Theorem 89, (5.12) with (5.13), the conditionals  $z_i|z_{-i}$  are compatible as a Besag auto-model with marginal distribution

$$\text{pr}_Z(z) \propto \exp \left( \overbrace{\sum_i \left( \underbrace{\alpha_i z_i}_{V_i(z_i)} + \underbrace{\log(z_i!)}_{C_i(z_i)} \right)}^{U(z)=} + \sum_i \sum_{j:j \sim i} \beta_{i,j} z_i z_j \right)$$

or otherwise the energy function is

$$U(z) = \sum_i (\alpha_i z_i + \log(z_i!)) + \sum_{j \sim i} \beta_{i,j} z_i z_j$$

Furthermore, to ensure that  $U(z)$  is admissible, we need to consider additional conditions. I observe that

$$\sum_{z \in \mathbb{N}^S} \exp(U(z)) = \sum_{z \in \mathbb{N}^S} \prod_i \left( \exp(\alpha_i z_i + \log(z_i!)) + \sum_{j \sim i} \beta_{i,j} z_i z_j \right)$$

- If we use additional condition  $\beta_{i,j} \leq 0$  then

$$\sum_{z \in \mathbb{N}^S} \exp(U(z)) \leq \sum_{z \in \mathbb{N}^S} \prod_i (\exp(\alpha_i z_i + \log(z_i!))) = \sum_{z \in \mathbb{N}^S} \prod_i \frac{1}{z_i!} \exp(\alpha_i z_i) < \infty$$

which converges. Modeling-wise,  $\beta_{i,j} < 0$  introduces competition among the neighbors similar to the Ising model. So by introducing a competition such as  $\beta_{i,j} \leq 0$  in the model I prevent the count  $z_i$  at  $i$  to explode.

- If  $\beta_{i,j} > 0$ , I discourage competition among neighboring sites. Admissibility can be satisfied if we truncate the state space as  $z_i < M$  for some fixed upper bound  $M$ . For instance, the characteristics  $z_i|z_{-i}$  can follow a Poisson distribution truncated at  $M$ .

$$\text{pr}_i(z_i|z_{-i}) = \frac{1}{z_i!} (\lambda_i(z_{-i}))^{z_i} \exp(-\lambda) 1(z_i \in \{0, 1, \dots, M\})$$

So I can prevent  $z_i$  at  $i$  to explode by forcefully bounding it  $z_i < M$  with a big enough value  $M > 0$ .

The resulting spatial model is called Poisson automodel.

*Note 92.* A CAR model is an automodel. Recall that CAR model is defined such as its local characteristics (full conditional distributions) are Gaussian distributions; however Gaussian distribution is an exponential distribution family. Hence the joint distribution of CAR model in Proposition 31 could have been derived from Theorem 83 as well.

### 5.3. Parameterization matters in automodels.

*Remark 93.* The unknown parameter vector  $\theta = ((\alpha_i; i \in \mathcal{S}), (\beta_{i,j}; i, j \in \mathcal{S}))$  in the automodel (5.1) (eg Besag's automodel (5.7)) can be further parameterised to have a particular structure without the need to consider any additional constraints in Theorem 83.

*Remark 94.* The dimensionality of  $\theta$  may be too large leading to an over-parameterized model or prohibitively large computational cost when the size of the set of sites  $\mathcal{S}$  is large (a usual case). To mitigate this issue, a way is to set a structure on  $\{\alpha_i, \beta_{i,j}\}_{i,j \in \mathcal{S}}$ , reducing its dimensionality.

- For instance, one may specify

$$\alpha_i = aw_i, \quad \text{and} \quad \beta_{i,j} = b_i c_j; \text{ for } i, j \in \mathcal{S},$$

with some known weights  $\{w_i; i \in \mathcal{S},\}$  and unknown  $\{a, b_i, c_j; i, j \in \mathcal{S}\}$ . Then learning  $\text{Card}(\mathcal{S}) (1 + \text{Card}(\mathcal{S}))$  unknown parameter  $\{\alpha_i, \beta_{i,j}; i, j \in \mathcal{S},\}$  reduces to learning just  $1 + 2\text{Card}(\mathcal{S})$  unknown parameters  $\{a, b_i, c_j; i, j \in \mathcal{S}\}$ . Note, that  $\beta_{i,j} = b_i c_j$  restricts the interaction between  $i, j$ .

*Remark 95.* When observable covariates  $x_i = (x_{i,1}, \dots, x_{i,p})^\top$  for  $i \in \mathcal{S}$  are available, one could “link” time to the model via the parameters  $\{\alpha_i, \beta_{i,j}\}_{i,j \in \mathcal{S}}$ , and make it time dependent.

- For instance by setting

$$(5.14) \quad \alpha_i = a_i + \sum_{k=1}^p d_k x_{i,k}, \quad \text{and} \quad \beta_{i,j} = \beta_{i,j}; \text{ for } i, j \in \mathcal{S},$$

where  $\{a_i; i \in \mathcal{S}\}$ ,  $\{d_k; k = 1, \dots, p\}$  and  $\{\beta_{i,j}; i, j \in \mathcal{S}\}$  are unknown parameters.  $d_k$  represents the influence of  $k$ -th covariate  $x_{i,k}$ , for all  $i \in \mathcal{S}$ .  $\beta_{i,j}$  represents the influence of the  $z_{\partial i}$  at the neighboring sites of  $Z_i$ . Examination of the sign of  $\beta_{i,j}$ , and  $d_k$  or whether  $\beta_{i,j} \neq 0$ ,  $d_k \neq 0$  facilitates the discovery of patterns and conditional dependencies.

*Remark 96.* Perhaps, in Remark 95, one (or many) of the observable covariates in vector  $x_i$  for  $i \in \mathcal{S}$  can be “time”  $t$  dependent. One could “link” them to the model via the parameters  $\{\alpha_i, \beta_{i,j}\}_{i,j \in \mathcal{S}}$ , and make the automodel dynamical (aka spatio-temporal).

- For instance, if one consider  $x_i = (t_i, t_i^2)^\top$  for  $i \in \mathcal{S}$  and set

$$\alpha_i = a_i + d_1 t_i + d_2 (t_i)^2, \quad \text{and} \quad \beta_{i,j} = \beta_{i,j}; \text{ for } i, j \in \mathcal{S},$$

essentially he/she makes the model dynamic (or space-time, or spatio-temporal)

Of course, how to parameterize the covariates in (5.14) is problem dependent, (similar to the linear regression) and a model assessment/comparison is often required.

**Example 97.** In Example 91, given observable covariates  $x_i = (x_{i,1}, \dots, x_{i,p})^\top$  for  $i \in \mathcal{S}$ , one may set (5.13) as

$$(5.15) \quad \log(\lambda_i(z_{-i})) = \left[ a_i + \sum_{k=1}^p d_k x_{i,k} \right] + \left[ \sum_{j:j \sim i} \beta_{i,j} z_j \right]$$

Then  $d_k$  represent the influence of  $k$ -th covariate  $x_{i,k}$ , for all  $i \in \mathcal{S}$ , and  $\beta_{i,j}$  represents the influence of the  $z_{\partial i}$  at the neighboring sites of  $Z_i$ . For admissibility, a condition such as  $\beta_{i,j} \leq 0$  should be specified (see Example 91). Further restrictions on the unknown parameters, or dimension reduction techniques, should be used because the number of unknowns is greater than the number of observations in (5.15).

**Example 98.** In Example 91, if the dataset is  $\{(t_i, s_i, Z_i); i \in \mathcal{S}\}$  where  $Z_i$  is the measurement (e.g. counts of a characteristic), at time  $t_i$ , at location  $s_i \in \mathbb{R}^2$  of the  $i$ -th observation, a researcher may consider a parametrization

$$(5.16) \quad \log(\lambda_i(z_{-i}, t_i)) = [a_i + d_1 t_i] + \left[ \sum_{j:j \sim i} \beta_{i,j} z_j \right]$$

and be interested in learning the unknown parameters  $\{a_i\}$ ,  $d_1$ , and  $\{\beta_{i,j}\}$ . Obviously, the resulted model is space-time.

## 6. FREQUENTIST MODELING AND LIKELIHOOD BASED INFERENCE

*Note 99.* Consider a dataset  $\{(s_i, Z_i = Z(s_i)); i = 1, \dots, n\}$  where  $Z_i$  is the observation at site  $s_i$  for  $i = 1, \dots, n$ . Assume that the sampling distribution of  $(Z_i)_{i=1}^n$  is specified by the researcher to be

$$(6.1) \quad Z \sim \text{pr}_Z(Z|\theta)$$

labeled by unknown parameter vector  $\theta$ . Parametric and predictive inference can be performed based on the associated likelihood or its approximation PsuedoLikelihood.



*Note 100.* For easy of presentation we assume that the observables  $Z$  are a realization of an automodel and hence their sampling distribution (6.1) is that of the automodel (5.1) with potentials 5.3 and 5.4, and unknown parameter  $\theta = (\{\alpha_i\}, \{\beta_{i,j}\})^\top$ .

### 6.1. MLE: Maximum likelihood estimation.

*Note 101.* We describe the maximum likelihood estimation in the automodel framework.

*Remark 102.* In the MLE framework, given a dataset  $\{(s_i, Z_i = Z(s_i)); i = 1, \dots, n\}$ , estimation of the unknown parameters  $\{\alpha_i\}$  and  $\{\beta_{i,j}\}$  of an automodel can be performed by maximizing the likelihood, as

$$(6.2) \quad \left( \{\hat{\alpha}_i\}, \{\hat{\beta}_{i,j}\} \right) = \arg \max_{\{\alpha_i\}, \{\beta_{i,j}\}} (\text{pr}_Z(Z | \{\alpha_i\}, \{\beta_{i,j}\}))$$

subject to  $\beta_{i,j} = \beta_{j,i}, \forall i, j \in \mathcal{S}$   
...and any other problem specific restrictions

where  $\text{pr}_Z(Z | \{\alpha_i\}, \{\beta_{i,j}\})$  is the joint distribution (5.7) given the unknown parameters  $\{\alpha_i\}$  and  $\{\beta_{i,j}\}$ .

**Example 103.** (Logistic automodel / Ising model) Assume that observables  $Z$  follow the Logistic automodel (5.11) in Example 90. Computing MLE  $\{\hat{\alpha}_i\}, \{\hat{\beta}_{i,j}\}$  of  $\{\alpha_i\}, \{\beta_{i,j}\}$  requires

$$(6.3) \quad \begin{aligned} \left( \{\hat{\alpha}_i\}, \{\hat{\beta}_{i,j}\} \right) &= \arg \max_{\{\alpha_i\}, \{\beta_{i,j}\}} (\log (\text{pr}_Z(Z | \{\alpha_i\}, \{\beta_{i,j}\}))) \\ &= \arg \max_{\{\alpha_i\}, \{\beta_{i,j}\}} \left( \sum_i \alpha_i z_i + \sum_{\{i,j\}: j \sim i} \beta_{i,j} z_i z_j - \log (C(\{\alpha_i\}, \{\beta_{i,j}\})) \right) \end{aligned}$$

where

$$(6.4) \quad C(\{\alpha_i\}, \{\beta_{i,j}\}) = \sum_{\forall z \in \mathcal{Z}^{\mathcal{S}}} \exp \left( \sum_i \alpha_i z_i + \sum_{\{i,j\}: j \sim i} \beta_{i,j} z_i z_j \right)$$

is the normalizing constant. Optimization in (6.3) can be done numerically by using a recursive optimization algorithm such as Newton-Raphson.

*Note 104.* The optimization problem (6.2) can be too computationally expensive. For instance, in Example 103, a recursive optimization algorithm, like Newton-Raphson, requires several iterations. At each iteration the evaluation of the (parameter dependent) constant (6.4) has to be evaluated. A computation of that constant can be too expensive when the set of sites  $i \in \mathcal{S}$  is large because the sum  $\sum_{\forall z \in \mathcal{Z}^{\mathcal{S}}}$  in (6.4) implies scanning all the possible

configurations of  $z \in \mathcal{Z}^S$ . A way to mitigate this is to use instead an “approximation” of the likelihood, such as the Pseudo-likelihood.

## 6.2. MPLE: Maximum pseudo likelihood estimation.

*Note 105.* We describe the maximum pseudo likelihood estimation in the automodel framework.

**Definition.** The pseudo likelihood  $\text{pseudo}L(Z; \theta)$  of observables  $Z = (Z_1, \dots, Z_n)^\top$  given parameters  $\theta$  is an approximation of the (exact) likelihood  $L(Z; \theta)$  of observables  $Z = (Z_1, \dots, Z_n)^\top$  given parameters  $\theta$  which is equal to

$$\text{pseudo}L(Z; \theta) = \prod_i \text{pr}(Z_i | Z_{-i}, \theta)$$

where  $\text{pr}(Z_i | Z_{-i}, \theta)$  are the conditionals of the joint pdf/pmf of the sampling distribution  $\text{pr}(Z | \theta)$  of  $Z$  given parameter  $\theta$ .

**Definition.** (Maximum PseudoLikelihood Estimator) The Maximum Pseudo-Likelihood Estimator (MPLE)  $\tilde{\theta}$  of  $\theta$  is the maximizer of the pseudo likelihood function  $\text{pseudo}L(Z; \theta)$  where the parameter  $\theta$  is the argument and the observables  $Z = (Z_1, \dots, Z_n)^\top$  are fixed values.

$$\tilde{\theta} = \arg \max_{\theta} (\text{pseudo}L(Z; \theta))$$

*Remark 106.* Then (6.2) becomes: In the MPLE framework, given a dataset  $\{(s_i, Z_i = Z(s_i)); i = 1, \dots, n\}$ , of the unknown parameters  $\{\alpha_i\}$  and  $\{\beta_{i,j}\}$  of an automodel can be performed by maximizing the pseudo-likelihood, as

$$(6.5) \quad \left( \{\hat{\alpha}_i\}, \{\hat{\beta}_{i,j}\} \right) = \arg \max_{\{\alpha_i\}, \{\beta_{i,j}\}} \left( \prod_{i \in \mathcal{S}} \text{pr}_Z(Z_i | Z_{-i}, \theta) \right)$$

$$(6.6) \quad = \arg \max_{\{\alpha_i\}, \{\beta_{i,j}\}} \left( \sum_{i \in \mathcal{S}} \log(\text{pr}_Z(Z_i | Z_{-i}, \theta)) \right)$$

subject to  $\beta_{i,j} = \beta_{j,i}, \forall i, j \in \mathcal{S}$

...and any other problem specific restrictions

**Example 107.** (Logistic automodel / Ising model) (Cont. Example 103) Assume that observables  $Z$  follow the Logistic automodel (5.11) in Example 90. From (5.10), the conditionals (local characteristics) are computed to be such as

$$\log(\text{pr}_i(z_i | z_{-i})) = z_i \left( \alpha_i + \sum_{j \sim i} \beta_{i,j} z_j \right) - \log \left( 1 + \exp \left( \alpha_i + \beta_{i,j} \sum_{j: j \sim i} \beta_{i,j} z_j \right) \right)$$

and hence

$$\begin{aligned} \left( \{\hat{\alpha}_i\}, \{\hat{\beta}_{i,j}\} \right) &= \arg \max_{\{\alpha_i\}, \{\beta_{i,j}\}} \left( \sum_{i \in \mathcal{S}} \log (\text{pr}_i(z_i | z_{-i})) \right) \\ &= \arg \max_{\{\alpha_i\}, \{\beta_{i,j}\}} \left( \sum_{i \in \mathcal{S}} z_i \left( \alpha_i + \sum_{j \sim i} \beta_{i,j} z_j \right) - \sum_{i \in \mathcal{S}} \log \left( 1 + \exp \left( \alpha_i + \beta_{i,j} \sum_{j: j \sim i} \beta_{i,j} z_j \right) \right) \right) \end{aligned}$$

which does not depend on the normalizing constant (6.4) and hence its computation is less computationally demanding.

## 7. HIERARCHICAL MODELING (BAYESIAN MODELING)

### 7.1. A general framework for the hierarchical modeling (A revision).

*Note 108.* Uncertainty in spatial statistics can be decomposed according to the Hierarchical spatial model

$$(7.1) \quad \begin{cases} Z|Y, \vartheta & \text{data model} \\ Y|\vartheta & \text{spatial process model} \end{cases}$$

with

$$\text{pr}(Z, Y | \vartheta) = \text{pr}(Z | Y, \vartheta) \text{pr}(Y | \vartheta)$$

**Data model:** expresses the measurement uncertainty as it is quantified via the distribution  $\text{pr}(Z | Y, \vartheta)$  possibly labeled by some parameter  $\vartheta$ . It is often specified/modeled so that it can measure the goodness of fit between  $Z$  and  $Y$ .

**Spatial process model:** expresses the scientific uncertainty (e.g., that coming from  $(Y_s)$ ) as it is quantified via the specified distribution  $\text{pr}(Y | \vartheta)$  possibly labeled by some parameter  $\vartheta$ . It is often specified/modeled with purpose (among others) to encourage spatial coherence and represent spatial dependence.

See for example Figure 7.1

*Note 109.* Let the unknown parameter vector be  $\vartheta = (\vartheta_1, \vartheta_2)^\top$ . Assume that a prior is specified for the unknown  $\vartheta_1$  as  $\vartheta_1 | \vartheta_2 \sim \text{pr}(\vartheta_1 | \vartheta_2)$  i.e.  $\vartheta_1$  is unknown and random. Assume  $\vartheta_2$  is a fixed parameter without a specified prior; it can be considered sometimes as known and sometimes as unknown in what follows. (!)

*Note 110.* Then the Bayesian spatial hierarchical model becomes

$$(7.2) \quad \begin{cases} Z|Y, \vartheta_1, \vartheta_2 & \text{data model} \\ Y|\vartheta_1, \vartheta_2 & \text{spatial process model} \\ \vartheta_1|\vartheta_2 & \text{hyper-parameter prior model} \end{cases}$$

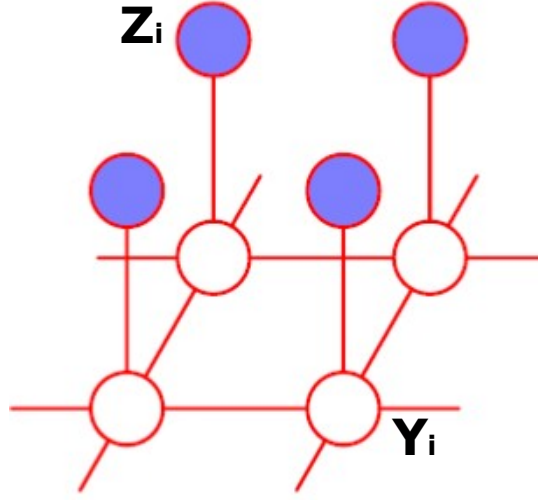


FIGURE 7.1. Hierarchical spatial model structure.  $\{Y_i\}$  is the spatial process model which is hidden.  $\{Z_i\}$  is the data model. The cartoon depicts a hierarchical spatial model with the special conditional independence structure  $Z_i | \{Y_i\}, \vartheta \sim \prod_i \text{pr}(Z_i | Y_i, \vartheta)$  and  $Y | \vartheta \sim \text{pr}(Y | \vartheta)$

where uncertainty is described by

$$\text{pr}(Z, Y, \vartheta_1 | \vartheta_2) = \text{pr}(Z | Y, \vartheta_1 | \vartheta_2) \text{pr}(Y | \vartheta_1, \vartheta_2) \text{pr}(\vartheta_1 | \vartheta_2)$$

*Note 111.* Under Bayesian model (7.2), when  $\vartheta_2$  is considered as unknown (but fixed),  $\vartheta_2$  can be learned pointwise by computing a point estimator  $\hat{\vartheta}_2$  as MLE i.e.

$$(7.3) \quad \hat{\vartheta}_2 = \arg \min_{\vartheta_2} (-2 \log (\text{pr}(Z | \vartheta_2)))$$

by maximizing the marginal likelihood

$$\text{pr}(Z | \vartheta_2) = \int \text{pr}(Z, Y, \vartheta_1 | \vartheta_2) dY d\vartheta_1$$

or as a MPLE

$$\tilde{\vartheta}_2 = \arg \min_{\vartheta_2} \left( -2 \log \left( \prod_i \text{pr}(Z_i | Z_{-i}, \vartheta_2) \right) \right)$$

by maximizing the pseudo marginal Likelihood

$$\text{pseudo}L(Z | \vartheta_2) = \prod_i \text{pr}(Z_i | Z_{-i}, \vartheta_2)$$

as a computational cheap approximation of the MLE  $\hat{\vartheta}_2$  in 7.3.

*Note 112.* Under Bayesian model (7.2), when  $\vartheta_1$  is considered as unknown (but random), namely, the a prior  $\vartheta_1 \sim \text{pr}(\vartheta_1 | \vartheta_2)$  has been specified, uncertainty about unknown  $\vartheta_1$  given

$Y$  and  $\vartheta_2$  can be represented by the posterior distribution

$$\text{pr}(\vartheta_1|Z, \vartheta_2 = \hat{\vartheta}_2) = \frac{\text{pr}(Z|\vartheta_1, \vartheta_2) \text{pr}(\vartheta_1|\vartheta_2 = \hat{\vartheta}_2)}{\text{pr}(Z|\vartheta_2 = \hat{\vartheta}_2)}$$

where the value  $\hat{\vartheta}_2$  is plugged in. Alternatively, we can plug-in  $\tilde{\vartheta}_2$ .

*Note 113.* General interest lies in computing the posterior distributions of the spatial process model  $(Y_i)_{i \in \mathcal{S}}$ , (or latent process, or noiseless process) given the data  $Z$

$$\text{pr}(Y|Z, \vartheta_2 = \hat{\vartheta}_2) = \int \text{pr}(Y|Z, \vartheta_2 = \hat{\vartheta}_2) \text{pr}(\vartheta_1|Z, \vartheta_2 = \hat{\vartheta}_2) d\vartheta_1$$

*Note 114.* The above statistical problem is naturally addressed in the (either full or empirical) Bayesian statistical framework.

*Note 115.* Below we give two examples in aerial data.

## 7.2. Examples.

7.2.1. *A simplified spatial model for binary data (e.g. Image denoising).*

**Example 116.** (Image denoising) A central aim in image processing is to reconstruct an object (e.g. image)  $Y = (Y_i; i \in \mathcal{S})$  based on a measurement (observation)  $Z = (Z_i; i \in \mathcal{S})$  which is contaminated by errors  $\varepsilon = (\varepsilon_i; i \in \mathcal{S})$ . The framework of hierarchical modeling for aerial spatial data is suitable to address such cases.

Consider the image restoration dataset in Example 23 in Handout 1: Types of spatial data. (Figure 7.2a) We have a black and white noisy image with size  $240 \times 320$  pixels.

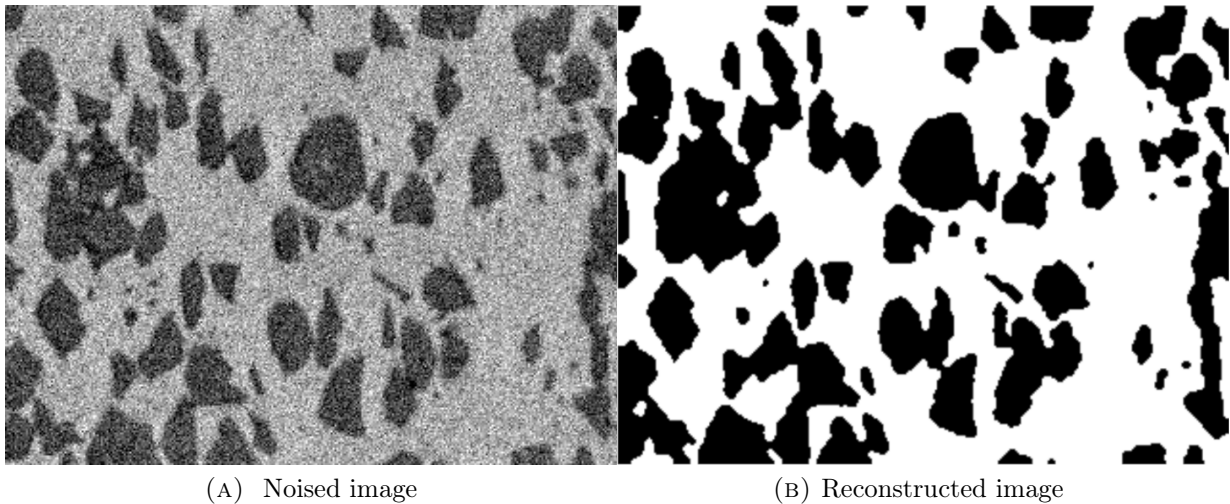


FIGURE 7.2. Ferrite-Pearlite steel image (Image restoration)

Mathematically, denote  $(Z_i)_{i \in \mathcal{S}}$  as the error contaminated (observed) image. The observables are coded as  $Z_i = 1$  for black and  $Z_i = 0$  for white at site  $i \in \mathcal{S} = \{1, \dots, 240 \times 320\}$ . Let  $n = \text{Card}(\mathcal{S})$ . Hence  $(Z_i)_{i \in \mathcal{S}}$  is a realization from the data model. The aim is to recover/learn the unknown real (error free) image  $(Y_i)_{i \in \mathcal{S}}$  given the measurement/observation  $(Z_i)_{i \in \mathcal{S}}$ .

The data model can be specified (for instance) by “assuming” that the observation  $Z_i$  has been contaminated by iid noise with some “probability”  $p$  for all pixels  $i \in \mathcal{S}$ ; i.e.  $p = \text{pr}(\{Z_i \neq Y_i\} | p) = 1 - \text{pr}(\{Z_i = Y_i\})$  for all  $i \in \mathcal{S}$ . Hence

$$\text{pr}(Z_i | Y_i, p) = p^{1-1(\{Z_i=Y_i\})} (1-p)^{1(\{Z_i=Y_i\})}, \quad i \in \mathcal{S}$$

Consequently, the data model is

$$\begin{aligned} \text{pr}(Z|Y, p) &= \prod_{i=1}^n p^{1-1(\{Z_i=Y_i\})} (1-p)^{1(\{Z_i=Y_i\})} = p^{n_{(Z,Y)}} (1-p)^{n-n_{(Z,Y)}} \\ &= \exp \left( n_{(Z,Y)} \log \left( \frac{p}{1-p} \right) + (1-p)^n \right) \end{aligned}$$

where  $n_{(Z,Y)} = \sum_{i \in \mathcal{S}} 1(\{Z_i = Y_i\})$ .

The spatial process  $(Y_i)_{i \in \mathcal{S}}$  is unknown (unobserved), and, according the Bayesian paradigm, we need to specify a prior process on  $(Y_i)_{i \in \mathcal{S}}$  account for the uncertainty. To introduce spatial dependence, the researcher may judge to specify (for example) an Logistic automodel (Ising model) process prior such as

$$\text{pr}(Y|\alpha, \beta) \propto \exp \left( \alpha \sum_{i \in \mathcal{S}} Y_i + \beta \sum_{\{i,j\}: i \sim j} Y_i Y_j \right), \quad \{0, 1\}^{\mathcal{S}}$$

with symmetric relation  $i \sim j$  considering only the adjacent pixels.

The researcher may be uncertain about the “real” value of  $p$  and hence he/she may want to specify a conjugate Beta prior<sup>2</sup>  $p \sim \text{Be}(g, h)$  with known  $g$  and  $h$  to account for the uncertainty. The researcher may set certain fixed values on  $\alpha$  and  $\beta$ ; hence consider that  $g$ ,  $h$ ,  $\alpha$ , and  $\beta$  are known values.

The Hierarchical Bayesian model is summarized as

$$(7.4) \quad \begin{cases} Z|Y, p \sim \text{pr}(Z|Y, p) & \text{data model} \\ Y \sim \text{pr}(Y|\alpha, \beta) & \text{spatial process model} \\ p \sim \text{Be}(g, h) & \text{hyper-parameter prior model} \end{cases}$$

---

<sup>2</sup> $\text{Be}(p|g, h) = p^{g-1} (1-p)^{h-1} 1_{(0,1)}(p) / \text{B}(g, h)$

To learn  $Y|Z$ , one can compute the Bayesian MAP estimator of  $Y$ , i.e.

$$\begin{aligned}\hat{Y} &= \arg \max_Y (\log (\text{pr} (Z|Y) \text{pr} (Z) / \text{pr} (Z))) \\ &= \arg \min_Y (-\log (\text{pr} (Z|Y)) - \log (\text{pr} (Y)))\end{aligned}$$

where

$$\begin{aligned}\text{pr} (Z|Y) &= \int p^{n(Z,Y)} (1-p)^{n-n(Z,Y)} \text{Be} (p|g, h) dp \\ &= \int p^{n(Z,Y)} (1-p)^{n-n(Z,Y)} \frac{p^{g-1} (1-p)^{h-1}}{\text{B} (g, h)} dp \\ &= \frac{1}{\text{B} (g, h)} \int p^{n(Z,Y)+g-1} (1-p)^{n-n(Z,Y)+h-1} dp \\ &= \frac{1}{\text{B} (g, h)} \text{B} (n(Z, Y) + g, n - n(Z, Y) + h)\end{aligned}$$

via an optimization numerical algorithm, or perhaps the posterior expectation, i.e.

$$\hat{Y} = \text{E} (Y|Z) = \int Z \text{pr} (Y|Z) dY$$

via MCMC, INLA, etc... Here the marginal posterior can be computed analytically as

$$\begin{aligned}\text{pr} (Y|Z) &= \int \text{pr} (Y, p|Z) dp = \int \frac{\text{pr} (Z|Y, p) \text{pr} (Y) \text{pr} (p)}{\int \text{pr} (Z|Y, p) \text{pr} (Y) \text{pr} (p) dp dZ} dp \\ &\propto \underbrace{\int \text{pr} (Z|Y, p) \text{pr} (p) dp}_{=\text{pr}(Z|Y)} \text{pr} (Y) = \text{pr} (Z|Y) \text{pr} (Y) \\ &\propto \underbrace{\frac{1}{\text{B} (g, h)} \text{B} (n_{(Z,Y)} + g, n - n(Z, Y) + h)}_{=\text{pr}(Z|Y)} \\ &\quad \times \underbrace{\frac{\exp \left( \alpha \sum_i Y_i + \beta \sum_{j \sim i} Y_i Y_j \right)}{\sum_{Y \in \{0,1\}^n} \exp \left( \alpha \sum_i Y_i + \beta \sum_{j \sim i} Y_i Y_j \right)}}_{=\text{pr}(Y)} \\ (7.5) \quad &\propto \text{B} (n(Z, Y) + g, n - n(Z, Y) + h) \exp \left( \alpha \sum_i Y_i + \beta \sum_{j \sim i} Y_i Y_j \right)\end{aligned}$$

Note that the only reason that we ignored the constant from the Ising process prior in (7.5) was because, in this particular example, the researcher considered  $\alpha$  and  $\beta$  as known constants. Of course, that constant should not have been ignored if  $\alpha$  and  $\beta$  had been considered as unknown, and hence we had to learn them.

Figure 7.2b shows the restored image as the Bayesian MAP estimator  $\hat{Y} = \arg \max_Y (\log (\text{pr}(Y|Z)))$  of  $Y|Z$  by using an R optimization function against (7.5).

### 7.2.2. A simplified spatial model for count data (e.g. Counts analysis).

**Example 117.** Consider the statistical problem scenario where there is available a dataset  $\{(X_i, s_i, Z_i); i = 1, \dots, n\}$ , where  $Z_i \in \mathbb{N}$  is the count of the occurrence of an event in a particular time interval, at a location  $s_i$ , and associated with a vector of covariates (other measurements)  $X_i = (X_{i,1}, \dots, X_{i,k})^\top$ , for  $i \in \mathcal{S}$ , with  $\mathcal{S} = \{1, \dots, n\}$ , and  $n \in \mathbb{N} - \{0\}$  fixed. So, denote  $(Z_i)_{i \in \mathcal{S}}$  as the observed vector. Assume that  $Z_i \in \mathcal{Z}^\mathcal{S}$ , with  $\mathcal{Z} = \mathbb{N}$  and  $\mathcal{S} = \{1, \dots, n\}$ .

- Such a scenario is suitable for the Columbus OH data set which concerns spatially correlated count data arising from small area sampling of some underlying process. This is the R dataset `columbus{spdep}`. Briefly, the Columbus data frame has 49 rows and 22 columns. Unit of analysis is 49 neighborhoods in Columbus, OH, 1980 data. The data frame has among others variables

**NEIG:** neighborhood id value (1-49); conforms to id value used in Spatial Econometrics book.

**CRIME:** residential burglaries and vehicle thefts per thousand households in the neighborhood

**HOVAL:** housing value (in 1,000 USD)

**INC:** household income (in 1,000 USD)

$$\left\{ \left( \underbrace{\text{HOVAL}_i, \text{INC}_i}_{X_i}, \underbrace{\text{NEIG}_i}_{s_i}, \underbrace{\text{CRIME}_i}_{Z_i} \right)^\top ; i = 1, \dots, \underbrace{49}_n \right\}$$

- Figure 2a shows the Property crime (number per thousand households) in 49 districts/neighborhood in Columbus in 1980, as well as the average value of the house in USD. Figure 2b presents the corresponding average house value. For privacy reasons, these are typically aggregated over areas that are large enough to ensure that the counts cannot be traced back to individuals.
- Interest may lie to find whether high rates of crime are clustered in a particular areas, and, perhaps what is the association of it with the value of the houses in the area.



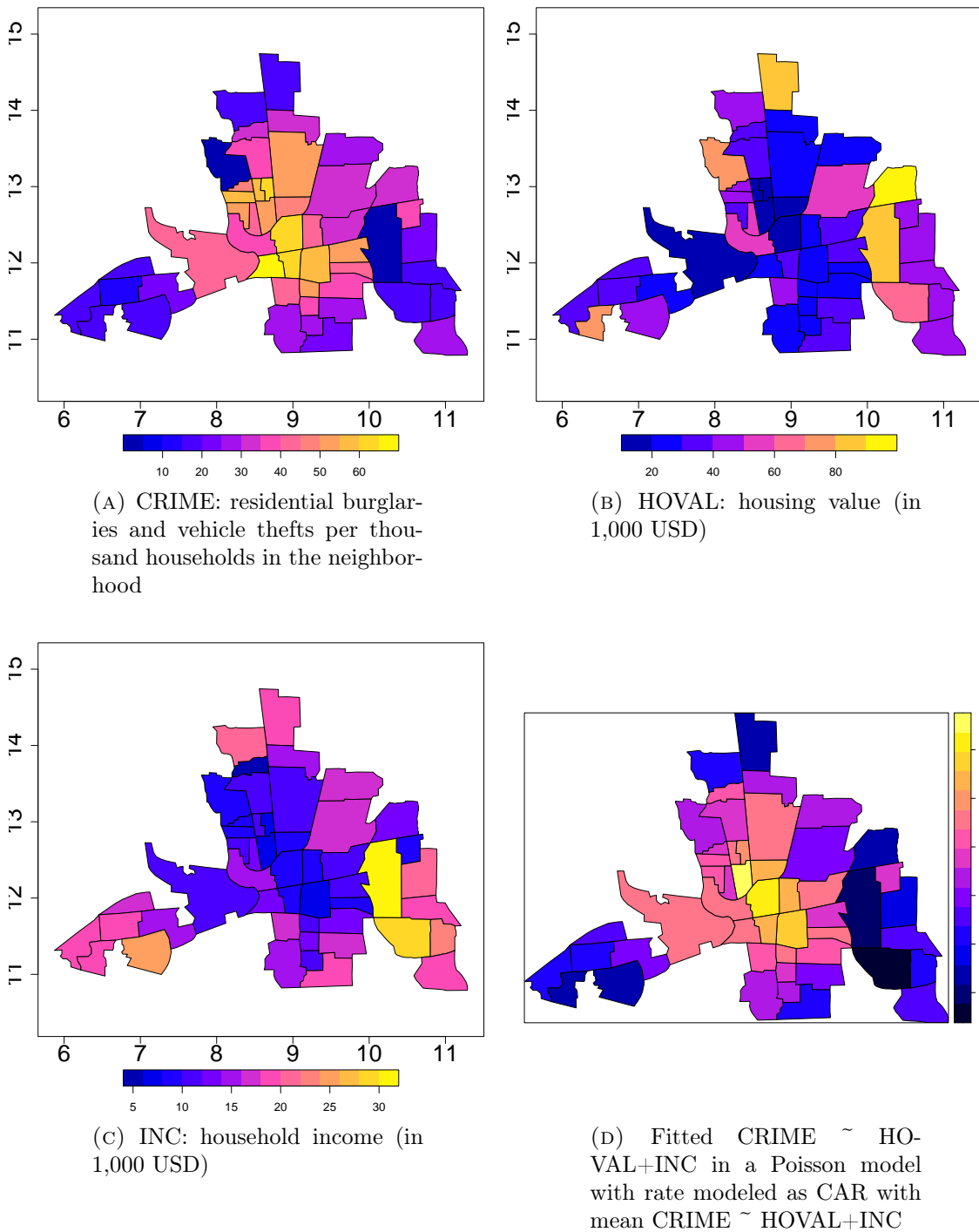


FIGURE 7.3. Columbus Columbus OH spatial analysis dataset

For the data model, it is natural to assume that for site  $s_i$  the observable count  $Z_i$  is sampled from a Poisson distribution with some given rate  $\lambda_i := \mathbb{E}(Z_i|Y_i) = \log(Y_i)$ , different for different sites  $s_i$  and depending on an unknown/unobserved and underpinning spatial

Page 33

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process  $(Y_i)_{i \in \mathcal{S}}$ . The researcher may specify the data model as

$$(7.6) \quad Z_i | Y_i \stackrel{\text{ind}}{\sim} \text{Poisson}(\lambda_i(Y_i)), \text{ for } i = 1, \dots, n$$

$$\text{where } \log(\lambda_i) = Y_i$$

This imposes the (rather strong) assumption that  $Z_i$  and  $Z_j$  are conditionally independent given the spatial process  $(Y_i)_{i \in \mathcal{S}}$ .

- For the Columbus dataset, data model (7.6) is reasonable because the observation  $Z_i$  represents count namely number of event in a specific time and space and with fixed rate  $\lambda_i$  for each individual neighborhood  $i \in \mathcal{S}$ .

The spatial process  $Y$  is unknown. To specify the uncertainty on  $Y$ , the researcher may judge to assign a CAR model prior on  $(Y_i)_{i \in \mathcal{S}}$ , for instance

$$(7.7) \quad Y_i | Y_{-i} \sim N(\mu_i + \beta_{i,j}(Y_j - \mu_j), \kappa_i), \text{ for } i = 1, \dots, n$$

$$\mu_i = X_i^\top \alpha.$$

To reduce parametric dimensionality, we impose a more restrictive structure such that  $\kappa_i = 1/\tau$  for all  $i = 1, \dots, n$ , and

$$\beta_{i,j} = \begin{cases} \phi & \text{if } i \sim j \\ 0 & \text{if } i \not\sim j \text{ or } i = j \end{cases}$$

- In the Columbus example we Spatial process (7.7) is suitable with regressors  $X_i = (1, \text{HOVAL}_i, \text{INC}_i)^\top$ ; that is  $\text{CRIME} \sim \text{HOVAL} + \text{INC}$ .

$$\mu_i = \alpha_0 + \alpha_1 \text{HOVAL}_i + \alpha_2 \text{INC}_i, \quad i = 1, \dots, n$$

This is because we are interested in investigating “whether high rates of crime (CRIME) are clustered in a particular areas ( $i \in \mathcal{S}$ ), eg areas with expensive houses (HOVAL), and if yes, perhaps what is the association of it with the value of the houses in the area (INC)”. Hence we can use our model in order to see the association of CRIME with SPACE (i.e.  $i \in \mathcal{S}$ ), HOVAL (i.e. house value), and INC (i.e. income).

- Note that unlike the usual linear model, here I have managed to introduce spatial dependence in the model as well by

$$\begin{aligned}
E(Y_i|Y_{-i}) &= \underbrace{\alpha_0 + \alpha_1 \text{HOVAL}_i + \alpha_2 \text{INC}_i}_{\text{cocariate dependence only}} + \underbrace{\sum_{i \sim j} \phi(Y_j - \mu_j)}_{\text{spatial dependence}} \\
&= \underbrace{\alpha_0 + \alpha_1 \text{HOVAL}_i + \alpha_2 \text{INC}_i}_{\text{cocariate dependence only}} + \underbrace{\sum_{i \sim j} \phi Y_j}_{\text{spatial dependence only}} \\
&\quad - \underbrace{\sum_{i \sim j} \phi [\alpha_0 + \alpha_1 \text{HOVAL}_j + \alpha_2 \text{INC}_j]}_{\text{interaction of space and covariates}}
\end{aligned}$$

This essentially produces a joint model (see Section 3.1 or just use Theorem 83)

$$Y \sim N(X\alpha, (I - \phi N)^{-1} \tau^{-1})$$

where  $N$  is an  $n \times n$  matrix with  $[N]_{i,j} = 1$  ( $\{i \sim j\}, i \neq j$ ), where  $\sim$  is defined to denote adjacent sites (or otherwise spatial locations sharing same borders).

For the unknown hyper-parameters  $\alpha$ ,  $\phi$  and  $\kappa$ , the researcher may consider hyper-priors  $\alpha \sim N(0, \Sigma_\alpha)$ ,  $\phi \sim U(0, \phi_{\max})$ , and  $\tau \sim \chi^2(\nu)$ ; the prior distributions here are chosen for demonstration. The rest hyper-parameters  $\Sigma_\alpha > 0$ ,  $\phi_{\max} \in \{\phi > 0 : I - \phi N \text{ is non singular}\}$ ,  $\nu > 0$  are considered as unknown fixed constants set by the researcher based on his/her subjective believes.

The Bayesian spatial hierarchical model becomes

$$(7.8) \quad \begin{cases} Z_i|Y_i \stackrel{\text{ind}}{\sim} \text{Poisson}(\exp(Y_i)), \forall i & \text{data model} \\ Y|\alpha, \phi, \tau \sim N(X\alpha, (I - \phi N)^{-1} \tau^{-1}) & \text{spatial process model} \\ \alpha|\tau \sim N(\mu_\alpha, \tau^{-1} \Sigma_\alpha) & \text{hyper-prior model} \\ \tau \sim \chi^2(\nu) & \text{hyper-prior model} \\ \phi \sim U(0, \phi_{\max}) & \text{hyper-prior model} \end{cases}$$

The joint probability model becomes

$$\begin{aligned}
\text{pr}(Z, Y, \alpha, \beta, \tau) &= \prod_{i \in \mathcal{S}} \text{pr}(Z_i|Y_i) \text{pr}(Y|\alpha, \phi, \tau) \text{pr}(\alpha|\tau) \text{pr}(\tau) \text{pr}(\phi) \\
&= \prod_{i \in \mathcal{S}} \text{Poisson}(Z_i|\exp(Y_i)) N(Y|X\alpha, (I - \phi N)^{-1} \tau^{-1}) \\
&\quad \times N(\alpha|\mu_\alpha, \tau^{-1} \Sigma_\alpha) \text{ChiSq}(\tau|\nu) U(\phi|0, \phi_{\max})
\end{aligned}$$

Interest lies in learning  $Y|Z$  which can be addressed for instance by the Bayesian MAP estimator

$$\hat{\lambda} = \arg \max_Y (\text{pr}(\lambda|Z))$$

or the posterior expectation estimator

$$\hat{\lambda} = E_{\text{pr}}(\lambda|Z) = E_{\text{pr}}(\exp(Y)|Z)$$

$\text{pr}(\lambda|Z)$  can be computed via random variable transformation from  $\text{pr}(Y|Z)$  which is given by the Bayesian theorem as

$$\text{pr}(Y|Z) = \int \text{pr}(Y, \alpha, \tau, \phi|Z) d\alpha d\tau d\phi$$

$$\text{pr}(Y, \alpha, \tau, \phi|Z) \propto \text{pr}(Z, Y, \alpha, \tau, \phi) = \text{pr}(Z|Y) \text{pr}(Y|\alpha, \tau, \phi) \text{pr}(\alpha|\tau) \text{pr}(\phi)$$

The above integration is analytically intractable, and hence its numerical computation can be performed by methods such as MCMC, INLA, etc...

Some marginal pdf/pmf

$$\begin{aligned} \text{pr}(Y, \alpha, \tau, \phi|Z) &\propto \text{pr}(Z, Y, \alpha, \tau, \phi) \\ &= \prod_{i \in \mathcal{S}} \text{Poisson}(Z_i | \exp(Y_i)) \text{N}(Y | X\alpha, (I - \phi N)^{-1} \tau^{-1}) \text{N}(\alpha | \mu_\alpha, \Sigma_\alpha \tau^{-1}) \\ &\quad \times \text{U}(\phi | 0, \phi_{\max}) \text{ChiSq}(\tau | \nu) \end{aligned}$$

and

$$\begin{aligned} \text{pr}(Y, \tau, \phi|Z) &\propto \int \text{pr}(Z, Y, \alpha, \tau, \phi) d\alpha \\ &= \int \prod_{i \in \mathcal{S}} \text{pr}(Z_i | Y_i) \text{pr}(Y | \alpha, \tau, \phi) \text{pr}(\alpha | \tau) \text{pr}(\tau) \text{pr}(\phi) d\alpha \\ &= \prod_{i \in \mathcal{S}} \text{pr}(Z_i | Y_i) \underbrace{\int \text{pr}(Y | \alpha, \tau, \phi) \text{pr}(\alpha | \tau) d\alpha}_{=\text{pr}(Y|\phi, \tau)} \text{pr}(\tau) \text{pr}(\phi) \\ &= \prod_{i \in \mathcal{S}} \text{Poisson}(Z_i | \exp(Y_i)) \text{N}(Y | X\mu_\alpha, \Sigma(\phi) \tau^{-1}) \text{ChiSq}(\tau | \nu) \text{U}(\phi | 0, \phi_{\max}) \end{aligned}$$

where

$$\begin{aligned} \text{pr}(Y|\phi) &= \int \text{pr}(Y|\alpha, \tau, \phi) \text{pr}(\alpha|\tau) d\alpha \\ &= \text{N}(Y | X\mu_\alpha, ((I - \phi)^{-1} + X\Sigma_\alpha X^\top) \tau^{-1}) \\ &= \text{N}\left(Y | X\mu_\alpha, \left((I - \phi N) + (I - \phi N) X (\Sigma_\mu^{-1} + X^\top (I - \phi N) X)^{-1} X^\top (I - \phi N)\right) \tau^{-1}\right) \\ &= \text{N}(Y | X\mu_\alpha, \Sigma(\phi) \tau^{-1}) \end{aligned}$$

where

$$\Sigma(\phi) = \left( (I - \phi N) + (I - \phi N) X (\Sigma_\mu^{-1} + X^\top (I - \phi N) X)^{-1} X^\top (I - \phi N) \right)$$

and

$$\begin{aligned} \text{pr}(Y, \phi|Z) &\propto \int \text{pr}(Z, Y, \tau, \phi) d\tau \\ &= \int \prod_{i \in \mathcal{S}} \text{pr}(Z_i|Y_i) \text{pr}(Y|\tau, \phi) \text{pr}(\tau) \text{pr}(\phi) d\alpha \\ &= \prod_{i \in \mathcal{S}} \text{pr}(Z_i|Y_i) \underbrace{\int \text{pr}(Y|\tau, \phi) \text{pr}(\tau) d\tau}_{=\text{pr}(Y|\phi)} \text{pr}(\phi) \\ &= \prod_{i \in \mathcal{S}} \text{Poisson}(Z_i | \exp(Y_i)) T\left(Y|X\mu_\alpha, \frac{1}{\nu}\Sigma(\phi), \nu\right) U(\phi|0, \phi_{\max}) \end{aligned}$$

because

**Hint::** The following definition is given:

A  $d$  dimensional random vector  $y$  follows a Student t distribution with degrees of freedom  $\nu$ , mean parameter  $\mu$ , and scale parameter  $\Sigma$  iff it can be represented as  $y = \mu + \sqrt{\nu/\xi}x$  results as  $\xi \sim \chi_\nu^2$ , and  $x \sim N(0, \Sigma)$ . It is denoted as  $y \sim T(\mu, \Sigma, \nu)$ . If  $\Sigma > 0$ , then  $x$  has pdf

$$T(y|\mu, \Sigma, \nu) = \frac{\Gamma((\nu + d)/2)}{\Gamma(\nu/2) \nu^{\frac{d}{2}} \pi^{\frac{d}{2}} |\Sigma|^{\frac{1}{2}}} \left( 1 + \frac{1}{\nu} (y - \mu)^\top \Sigma^{-1} (y - \mu) \right)^{-\frac{\nu+d}{2}}$$

$$\begin{aligned} \text{pr}(Y|\phi) &= \int \text{pr}(Y|\phi, \tau) \text{pr}(\tau) d\tau \\ &= \int N(Y|X\mu_\alpha, \Sigma(\phi) \tau^{-1}) \text{ChiSq}(\tau|\nu) d\tau \\ &= \int N\left(Y|X\mu_\alpha, \Sigma(\phi) \tau^{-1} \frac{1}{\nu} \nu\right) \text{ChiSq}(\tau|\nu) d\tau \\ &= \int N\left(Y|X\mu_\alpha, \frac{\nu}{\tau} \left(\frac{1}{\nu} \Sigma(\phi)\right)\right) \text{ChiSq}(\tau|\nu) d\tau \\ &= \int N\left(Y|X\mu_\alpha, \frac{\nu}{\tau} \left(\frac{1}{\nu} \Sigma(\phi)\right)\right) \text{ChiSq}(\tau|\nu) d\tau \\ &= T\left(y|X\mu_\alpha, \frac{1}{\nu} \Sigma(\phi), \nu\right) \end{aligned}$$

Notice that

$$\text{pr}(Y|Z) = \int \text{pr}(Y, \phi|Z) d\phi$$

involves an analytically intractable one-dimensional integral which can be easily approximated by using a standard integration algorithm (e.g. parallelogram rule).

- In Columbus example, the resulted Bayesian hierarchical model is as in (7.8). Estimation was facilitated via INLA. The estimates are computed as the posterior expected values given the data  $Z$  as

$$\hat{\alpha} = \begin{pmatrix} \hat{\alpha}_{\text{const}} \\ \hat{\alpha}_{\text{HOVAL}} \\ \hat{\alpha}_{\text{INC}} \end{pmatrix} = \begin{pmatrix} 54.3139189 \\ -0.2821969 \\ -0.9882862 \end{pmatrix}$$

$\hat{\phi} = 0.1589004$ , and  $\hat{\kappa} = 87.65$ . The fitted counts  $\hat{Y}$  are presented in Figure 7.3d.

By comparing Figure 7.3a and Figure 7.3d, we see that there are certain locations where the fitted counts  $\hat{Y}$  and  $Z$  are substantially different. Perhaps, we could improve our parameterization in (7.7) by considering a less restrictive  $\beta_{i,j}$  or by including more covariates in the mean  $\mu_i$ .

*Remark 118.* Example 117 demonstrates that if INLA is used to facilitate inference in this particular model there is no reason to approximate  $\text{pr}(Y|Z, \phi)$  as  $\tilde{\text{pr}}_{\text{G}}(Y|Z, \phi)$  (e.g. by Laplace approx.) because it is

$$\text{pr}(Y|Z, \phi) \propto \text{pr}(Y, \phi|Z) \propto \prod_{i \in \mathcal{S}} \text{Poisson}(Z_i | \exp(Y_i)) \text{T}\left(Y | X\mu_{\alpha}, \frac{1}{\nu}\Sigma(\phi), \nu\right)$$

Hence, as discussed in Note 18 of the “Handout 2: Introduction to INLA & R-INLA”, the approximation step 3 in Algorithm 17 is omitted and the associated approximation error does not exist!

**Proposition 119.** *Following, we show that any SAR model can be written as a CAR model, however the inverse is not always true.*

*Proof.* Let  $\Lambda$  be  $n \times n$  positive diagonal matrix. Let  $\tilde{B}$  be  $n \times n$  positive matrix where  $I - \tilde{B}$  is non-singular and  $\tilde{B}_{i,i} := [\tilde{B}]_{i,i} = 0$ . Then  $(I - \tilde{B})^{-1} \Lambda (I - \tilde{B}^\top)^{-1}$  is well defined and I need to solve wrt  $B$  and  $K = \text{diag}(\kappa_1, \dots, \kappa_n)$

$$\begin{aligned} (I - B)^{-1} K &= (I - \tilde{B})^{-1} \Lambda (I - \tilde{B}^\top)^{-1} \Leftrightarrow \\ K^{-1} (I - B) &= (I - \tilde{B}^\top) \Lambda^{-1} (I - \tilde{B}) \Leftrightarrow \\ K^{-1} - K^{-1} B &= \Lambda^{-1} - \tilde{B}^\top \Lambda^{-1} - \Lambda^{-1} \tilde{B} + \tilde{B}^\top \Lambda^{-1} \tilde{B} \end{aligned}$$

If I focus of the diagonal part and set  $B_{i,i} := [B]_{i,i} = 0$

$$[K^{-1}]_{i,i} - \cancel{[K^{-1}B]_{i,i}} \stackrel{=0}{=} [\Lambda^{-1}]_{i,i} - \cancel{[\tilde{B}^\top \Lambda^{-1}]_{i,i}} \stackrel{=0}{=} \cancel{[\Lambda^{-1} \tilde{B}]_{i,i}} + \cancel{[\tilde{B}^\top \Lambda^{-1} \tilde{B}]_{i,i}}$$

so

$$\kappa_i = \left( \frac{1}{\lambda_i} + \sum_{j=1}^n \frac{\tilde{B}_{j,i}^2}{\lambda_j} \right)^{-1} > 0, \quad \forall i = 1, \dots, n$$

and hence I can solve with respect to  $K$  and  $B$  in a manner that they satisfy the assumptions of CAR.  $\square$

*Remark 120.* The converse of Proposition 119 is not true.