FAMILY BASED SPATIAL CORRELATION MODEL

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Family Based Spatial Correlation Model

by

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Abstract

In spatial data analysis, linear, count or binary responses are collected from a large sequence of (spatial) locations. This type of responses from the (spatial) locations may be influenced by certain fixed covariates associated to the location itself as well as certain invisible random effects from the members of the neighboring locations. Also the responses may be subject to certain model errors. In familial/clustered setup, responses are collected from the members of a large number of independent families, where the pairwise responses within the family are correlated. In a spatial set up, the pairwise responses within a family of locations are correlated similar to the familial setup, but unlike in the familial setup, the responses from neighboring families will also be correlated. In this thesis, unlike in the existing studies, we develop a moving or band correlation structure that reflects the correlations for within and between families. This is done first for linear (continuous) data and then for binary responses. As far as the inference are concerned, we discuss method of moments (MM) and

maximum likelihood (ML) approach for the estimation of parameters in linear mixed model setup. Because the exact likelihood estimation approach for the spatial binary models is complicated, we demonstrate how to use the generalized quasi-likelihood (GQL) approach for such models.

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Introduction

1.1 Motivation of the Problem

Over the last two decades, analysis of spatial data has become an emerging area of research in many different fields, such as ecology, environmental science, epidemiology, geography, sociology or economics and forestry. The spatial data are realizations of random variables collected from a sequence of related geographical locations, where the responses collected from adjacent locations naturally become correlated. These correlations are referred to as *spatial correlations*. Note that a response from a given location is usually influenced by certain fixed covariates apart from some invisible, say random effects associated to this and other adjacent locations. It is of interest to find the effects of the covariates after taking the spatial correlations of the responses into account. For various modeling for correlations and analysis of spatial data, we, for example, refer to Cressie (1993), and Gaetan and Guyon (2010).

Note that for a continuous spatial responses, the spatial correlations have been modeled so far either by using certain dynamic relationship among the errors in a linear model, such as time series type ARMA error process (Basu and Reinsel 1994, eqs. (1)-(2), p. 89), or by using a mixed model approach where responses are assumed to be influenced by certain correlated random effects referred to as *Spatial Random Process* as well as suitable independent errors (Kang, Cressie and Shi (2010), eqs.(7)-(19), p. 274 - 275, and Jones and Vecchia (1993), eq. (11), p. 949). For more on mixed model type spatial correlation processes, see also Cressie (1993, Chapter 3) and Gaetan and Guyon (2010, Section 1.8). Note, however, that there is no unique way to model the spatial correlations of the responses collected from neighboring locations. Because of the fact that any two responses collected from locations which are far apart are likely to be uncorrelated, using ARMA type spatial errors those considered by Basu and Reinsel (1994), for example, does not appear to be appropriate, as ARMA process based correlation may not die even when lags between the responses are moderately large or large. Remark that an MA type spatial process could be appropriate to model such correlations where correlations may be completely absent for a large lag.

Let there be S locations for a spatial problem. For $s = 1, 2, \cdots, S$, let y_s be the response on a continuous scale collected from the s^{th} location. Also, let $x_s = (x_{s1}, \cdots, x_{sp})'$ be the p dimensional fixed covariate vector corresponding to y_s and $\beta = (\beta_1, \cdots, \beta_p)'$ be the effect of x_s on y_s. Further suppose that apart from x_s, y_s be also influenced by an unobservable random effect γ_s. Jones and Vecchia (1993, eq. (11), p. 949) have used a linear mixed model to examine the effects of x_s on y_s. Their model is given by

$$y_s = x_s'\beta + \gamma_s + \epsilon_s, \quad \text{for} \quad s = 1, \cdots, S, \tag{1.1.1}$$

where, ϵ_s for $s = 1, \cdots, S$ are model errors and assumed to be independent. That is

$$\epsilon_s \stackrel{iid}{\sim} (0, \sigma_\epsilon^2). \tag{1.1.2}$$

As far as the random effects are concerned, Jones and Vecchia (1993) assumed that $\gamma_1, \cdots, \gamma_S$ are correlated with covariance matrix for $\gamma = (\gamma_1, \cdots, \gamma_S)'$ as

$$\text{cov}(\gamma) = \sigma_\gamma^2 C, \tag{1.1.3}$$

C being the $S \times S$ correlation matrix denoted as

$$C = (c_{sk}) : \quad S \times S, \tag{1.1.4}$$

with $c_{sk} = 1$ for $s = k$. In matrix notation this model (1.1.1) can be written as

$$y = X\beta + \gamma + \epsilon, \quad (1.1.5)$$

where $\text{Cov}(\gamma) = \sigma_\gamma^2 C$, $\text{Cov}(\epsilon) = \sigma_\epsilon^2 I_S$ and the elements of γ and ϵ are independent.

Next by writing

$$\sigma_\gamma^2 V = \sigma_\gamma^2 \left(C + \sigma_0^2 I_S\right), \quad (1.1.6)$$

with $\sigma_0^2 = \frac{\sigma_\epsilon^2}{\sigma_\gamma^2}$, Jones and Vecchia (1993) have estimated the parameters using the maximum likelihood approach. More specifically for known structure for V, they maximize the log likelihood function, that is, minimize

$$-2\log L = S\ln(2\pi\sigma_\gamma^2) + \ln \mid V \mid + \frac{1}{\sigma_\gamma^2}(y - X\beta)'V^{-1}(y - X\beta), \quad (1.1.7)$$

for the estimation of regression parameter β and the variance of the random effect σ_γ^2. When V is known, that is C and σ_ϵ^2 are known, the maximum likelihood estimates of these parameters (β and σ_γ^2) are given by

$$\hat{\beta} = (X'V^{-1}X)^{-1}(X'V^{-1}y)$$
$$\hat{\sigma}_\gamma^2 = \frac{1}{S}(y - X\hat{\beta})'V^{-1}(y - X\hat{\beta}). \quad (1.1.8)$$

Note that, to model the covariance structure V, Jones and Vecchia (1993) have used a class of stochastic linear partial differential equations. More specifically, the pair-wise covariances between two responses corresponding to, say, s^{th} and k^{th} locations separated by a distance r, has been modeled as

$$v_{sk} = g(\sigma_\epsilon^2, \sigma_0^2, \phi^*, \delta^*, r) \tag{1.1.9}$$

where, g is a known function in terms of a modified Bessel function of the second kind order 1 (see eqn. (6) in Jones and Vecchia (1993) , p. 948) and two additional parameters ϕ^* and δ^* arising from the partial differential equation. This approach appears to have several pitfalls. First it seems appropriate to use the covariance form (1.1.9) to model the C matrix in (1.1.6) instead of the V matrix. Furthermore, this form in (1.1.9) is equivalent to time domain based ARMA(p, q) process which may or may not yield uncorrelated random effects even if lag is large, whereas it is practical to assume that the C matrix contains correlations those die out completely where two responses are taken from a moderately large distant locations. Some authors such as Cressie (1991, p. 85-86) have used exponential or say Gaussian covariance function which is dependent on the distance (r) between two objects yielding zero correlation when the distance is large. In Jones and Vecchia's case, the correlation function may die even slower than that of the exponential correlation function considered by Cressie (1991). We however feel that the correlations obtained from two reasonably far apart distance responses should be zero, which require new modeling.

Basu and Reinsel (1994) consider regression models for spatial data that are observed on a two dimensional regular grid along with other explanatory variables, and the errors. Specifically they examined regression models with spatially correlated errors, have the marginal spatial response at site s (indexed by say, coordinates i and j) is modeled as:

$$y_s = x_s'\beta + \epsilon_s, \quad \text{for} \quad s = 1, \cdots, S. \tag{1.1.10}$$

Note however that ϵ_s's, for $s = 1, \cdots, S$ are correlated and follow a spatial unilateral first order ARMA model. By using a spatial cluster form with $Y = (y_1, \cdots, y_S)'$, $\epsilon = (\epsilon_1, \cdots, \epsilon_S)'$ and $X = (x_1, \cdots, x_S)'$, the regression model (1.1.10) can be written as

$$Y = X\beta + \epsilon, \tag{1.1.11}$$

where, the elements of vector ϵ is assumed to satisfy the spatial unilateral first order ARMA$(3,3)$ model given by

$$\begin{aligned}\epsilon_s &= \tilde{\alpha}_1\epsilon_{s-1} + \tilde{\alpha}_2\epsilon_{s-2} + \tilde{\alpha}_3\epsilon_{s-3} \\ &\quad +\tilde{\theta}_1\vartheta_{s-1} + \tilde{\theta}_2\vartheta_{s-2} + \tilde{\theta}_3\vartheta_{s-3} + a_s,\end{aligned} \tag{1.1.12}$$

where, $\vartheta_1, \cdots \vartheta_S$ are assumed to be independent with mean 0 and common variance σ_ϑ^2, and $a_s \overset{iid}{\sim} (0, \sigma_a^2)$. In (1.1.12), $\tilde{\alpha}_j$ and $\tilde{\theta}_j$ for $j = 1, 2, 3$ are referred to as autoregressive and moving average parameters respectively. Note that this spatial correlation modeling by (1.1.12) is similar to that of the correlation structure (1.1.9) considered by Jones and Vecchia (1993). The difference between these two models is that Jones and Vecchia (1993) used spectral density approach whereas Basu and Reinsel (1994) used a time domain approach. Note however that using ARMA type correlation structure may be reasonable when spatial objects are equally spaced (that is, maintain equal distance from each other).

There also exist some studies where correlations are modeled for extended spatial temporal data. For example, we refer to the recent article by Kang, Cressie and Shi (2010). At a given time $t = 1$, say, their spatial model (Kang, et. al.,(2010) eqn. (7), p. 274) has the form

$$\begin{aligned} y_s &= \mu_s + v_s + \xi_s + \epsilon_s \\ &= x_s'\beta + w_s'\gamma + \xi_s + \epsilon_s, \quad \text{for} \quad s = 1, \cdots, S, \end{aligned} \tag{1.1.13}$$

where, x_s' is the p dimensional covariate collected for s^{st} location, w_s is a vector of q dimensional known deterministic spatial basis functions and γ is a q dimensional vector of random effects with zero mean vector and $q \times q$ covariance matrix. Note that $\mu_s = x_s'\beta$ is usually referred to as a trend function and $v_s = w_s'\gamma$ is a function of unobservable random effects. Also in (1.1.13), $\xi_s \stackrel{iid}{\sim} (0, \sigma_\xi^2)$ and $\epsilon_s \stackrel{iid}{\sim} (0, \sigma_\epsilon^2)$ are referred to as the finite scale random component and measurement (or model) error, respectively. As opposed to the spatial temporal case, these ξ_s and ϵ_s are not identifiable in the spatial-only model (Cressie and Johannesson (2008)). Thus, in spatial setup, this (1.1.13) model is simplified as

$$y_s = x_s'\beta + w_s'\gamma + \epsilon_s^*, \quad \text{for} \quad s = 1, \cdots, S, \tag{1.1.14}$$

where, $\epsilon_s^* \stackrel{iid}{\sim} (0, \sigma_{\epsilon^*}^2)$. Remark that Kang et. al. (2010) have chosen the q dimensional random effect vector γ for all locations $s = 1, \cdots, S$ which may be appropriate only in some spacial cases such as when spatial locations are designed in a planned experiment with equal distances among locations following a linear pattern say. Also it is not clear how the value of q is chosen. Furthermore, it is also not clear how the w_s vector is chosen in practice. As opposed to these choices for q members of random effects at a location, it seems to be more practical to have a scheme where q_s random effects can be used for the s^{th} location which will allow a more general variable design involving unequal member of random effects over the locations. Similarly, a suitable scheme for the choice of w_s is also needed.

Note that in some situations spatial data are collected in the form of binary responses. For example, we refer to Rathbun and Cressie (1994, Section 5.2) for the modeling of tree mortality data in spatial-temporal setup. Here survival of a tree is considered as a binary response and the responses would exhibit two way correlations. However, when responses are considered in a spatial setup, only the binary response for a tree is likely to be correlated with other neighboring binary responses, but would not be correlated with responses from far distant locations. These correlations are in general caused by some common invisible random factors shared by pairwise trees. However modeling such correlations is not so easy. For common covariates based correlation modeling we refer to the model studied by Rathbun and Cressie (1994, eqns. (16) - (17)).

1.2 Objective of the Thesis

In spatial setup, where responses, whether linear, count or binary, are collected from different locations under a selected region, these responses are in general influenced by covariates associated to the location as well as certain common random factors shared by neighboring locations. Unlike in the temporal setup where responses are collected repeatedly from a given location, the modeling of correlations for spatial responses is not so straightforward. This is because spatial responses from neighboring locations are likely to be correlated but when moved to a far distant, the pairwise correlations are likely to be zero. It is naturally difficult to maintain this moving nature for correlations. Most of the existing studies explained in the last section, however, use temporal type relationships among spatial responses and correlations are modeled accordingly. There also has been the use of random effects to study their influence on the spatial responses (Kang et. al., (2010)) but modeling for spatial correlations among neighboring responses is not adequately discussed.

1. In Chapter 2, we propose a linear mixed model where weighted average of random effects from the member locations of a family is used to model the neighbor effects on a spatial response. When these random effects are independent, the model reduces to the well known linear mixed model in generalized linear model (GLM) setup. However, when random effects are correlated (usually equi-correlated) proposed model yields a familial correlation pattern for the correlations between members of two adjacent families. For simplicity, a special spatial linear pattern is considered to illustrate the spatial correlations.

2. In Chapter 3, we demonstrate how to apply the well-known method of moments (MM) and maximum likelihood (ML) approach to obtain consistent and efficient

regression estimates. Estimation of the scale and correlation parameters are also discussed. A simulation study is also given.

3. Unlike the linear mixed model cases, the spatial models for binary responses are not adequately addressed in the literature. We carry out the concept of weighted random effects used in linear mixed model case in Chapters 2 and 3, to the binary case and propose a new spatial correlation model for binary responses in Chapter 4. Following the existing generalized quasi-likelihood (GQL) estimation approach developed for generalized linear mixed models (GLMM), we develop marginal GQL estimating equations for all parameters including regression effects, variance of random effects, and pairwise correlation of random effects.

Chapter 2

Spatial Linear Mixed Models

In Section 1.1 we have reviewed the existing studies involving spatial analysis in linear mixed model setup. Most of these studies model the spatial correlation using temporal dynamic relationship. In this chapter, we propose a new familial random effects based spatial correlation model and deal with its marginal and correlation properties.

2.1 Proposed Spatial Linear Mixed Model

Consider a region $\mathcal{S}$ containing S spatial locations following a suitable design to be discussed below. Let y_s be the response at the s^{th} $(s = 1, \cdots, S)$ location, where this response may be influenced by a multi dimensional fixed covariate vector $x_s = (x_{s1}, \cdots, x_{sp})'$ containing the epidemiological and environmental information from the s^{th} location, as well as by some random effects belonging to a cluster of size n_s. We denote this cluster of random effects by a vector $\widetilde{\gamma}_s = (\widetilde{\gamma}_{s1}, \cdots, \widetilde{\gamma}_{sj_s} \cdots, \widetilde{\gamma}_{sn_s})'$. For the purpose of construction of $\widetilde{\gamma}_s$, we first define the s^{th} cluster, that is, the neighborhood of s^{th} location as follows.

Suppose that d^*_{sk} denote the Euclidian distance between the centers of the s^{th} spatial location and k^{th} (any other) location. Also suppose that d^* denotes a distance such that it is not necessary to seek for spatial correlations between the random effects of two locations apart from each other by a distance more than d^*. We now define an indicator variable δ_{sk} such that

$$\delta_{sk} = \begin{cases} 1 & \text{if} \quad d^*_{sk} \leq d^* \quad \text{for} \quad k = 1, \cdots, S \\ 0 & \text{otherwise,} \end{cases} \tag{2.1.1}$$

and the neighborhood of the s^{th} location, that is, the s^{th} cluster is formed with all locations satisfying (2.1.1). Let f_s be this cluster or family of locations. For the s^{th} cluster with size n_s, (say), it follows from (2.1.1) that

$$\sum_{k=1}^{S} \delta_{sk} = n_s. \tag{2.1.2}$$

Suppose that the individual random effects of all S locations are denoted by $\gamma_1^*, \cdots, \gamma_S^*$. Now for $s = 1, \cdots, S$ we assume that

$$\gamma_s^* \sim (0, \sigma_\gamma^2) \tag{2.1.3a}$$

and

$$\text{corr}(\gamma_r^*, \gamma_s^*) = \delta_{rs}\phi_{rs}^*. \tag{2.1.3b}$$

Also suppose that γ_{sk} denotes the random effect of the k^{th} location that belongs to s^{th} cluster or family satisfying (2.1.1). That is, for any k $(= 1, \cdots, S)$

$$\gamma_{sk} = \gamma_k^* \;\text{ for }\; k \in f_s. \tag{2.1.4}$$

Note that when $k = s$, $\gamma_{ss} = \gamma_s^*$ denotes the random effect of the s^{th} location around which the s^{th} family is constructed. Next because $\sum_{k=1}^{S} \delta_{sk} = n_s$ by (2.1.1), there are only n_s locations with random effects satisfying (2.1.4). We relabel or rearrange the n_s random effects γ_{sk} of the s^{th} family with $k \in f_s$ for

$$\widetilde{\gamma}_s = (\widetilde{\gamma}_{s1}, \cdots, \widetilde{\gamma}_{sj_s} \cdots, \widetilde{\gamma}_{sn_s})', \tag{2.1.5}$$

where, without any loss of generality, we use $\widetilde{\gamma}_{s1}$ in (2.1.5) to represent γ_{ss} from (2.1.4), that is,

$$\widetilde{\gamma}_{s1} \;=\; \gamma_{ss} \;=\; \gamma_s^*, \tag{2.1.6}$$

is the random effect of the center location. The remaining $n_s - 1$ random effects in (2.1.5) will be identified from (2.1.4) in a convenient way depending on the problem of interest.

Recall that in addition to x_s, the response y_s at s^{th} location/cluster is also influenced by the invisible random effects of s^{th} and other $n_s - 1$ neighboring locations. These random effects are the components of $\widetilde{\gamma}_s$ as defined in (2.1.5). Note that these random effects $\widetilde{\gamma}_{sj_s}$ for $j_s = 1, \cdots, n_s$ may be independent or correlated depending on the correlation structure of γ_k^* and the s^{th} family structure containing γ_k^* for $k \in f_s$. Furthermore, whether the random effects are independent or correlated, they will change the variance of the response y_s. They also will cause correlation between y_s and y_k for $s \neq k$, $s, k = 1, \cdots, S$, when the s^{th} and k^{th} locations are influenced by some common random effects. If the responses are continuous, one may then use a suitable linear mixed model for the response y_s at the s^{th} location. We propose this mixed model as

$$y_s \;=\; x_s'\beta + \frac{1}{\sqrt{n_s}} 1_{n_s}' \widetilde{\gamma}_s + \epsilon_s, \quad \text{for} \quad s = 1, \cdots, S \tag{2.1.7}$$

where, ϵ_s denotes the model error at the s^{th} location. We assume that $\epsilon_s \overset{iid}{\sim} (0, \sigma_\epsilon^2)$. In (2.1.7), β is the effect of fixed covariates x_s on y_s, and $1_{n_s} = (1, \cdots, 1)'$ is the $n_s \times 1$ unit vector. Note that the proposed model (2.1.7) is similar to (1.1.14) considered by

Kang et al. (2010). The difference between the two models is that the w_s in (1.1.14) is a subjective spatial basis function and the components of γ may or may not be associated with any spatial locations, whereas in (2.1.7) the components of $\widetilde{\gamma}_s$ are identified as the random effects of the neighboring locations belonging to s^{th} family. Also, we use $w_s = 1'_{n_s}/\sqrt{n_s}$ as a weight vector for $\widetilde{\gamma}_s$ constructed based on the number of random effects in the s^{th} family of locations for the following reasons:

1. If $1'_{n_s}\widetilde{\gamma}_s$ is used to understand the influence of the random effects of the neighboring locations, then these additive model produce

$$\text{var}\left(1'_{n_s}\widetilde{\gamma}_s\right) = n_s\sigma^2_\gamma,$$

   when random effects are independent. However this model can produce infinity or large variance for a responses when n_s is large, which does not appear to be practical.

2. An average of these random effects that is, $\dfrac{1}{n_s}1'_{n_s}\widetilde{\gamma}_s$ could yield the variance as

$$\text{var}\left(\frac{1}{n_s}1'_{n_s}\widetilde{\gamma}_s\right) = \frac{\sigma^2_\gamma}{n_s},$$

   which is again not practical as it will go to zero when $n_s \to 0$.

3. Because of the above two difficulties we consider $\dfrac{1}{\sqrt{n_s}}1'_{n_s}\widetilde{\gamma}_s$ as a weight function such that when random effects are independent the var $\left(\dfrac{1}{\sqrt{n_s}}1'_{n_s}\widetilde{\gamma}_s\right) = \sigma^2_\gamma$ which

is same as the variance of the individual random effect.

4. The advantage of using such weights is that the effects of correlation among random effects will be easily understood in the variance as well as covariance of the responses.

5. Note however that in some situations it may be reasonable to use a general weight pattern as

$$w_{s1} \geq w_{s2} \geq \cdots \geq w_{sn_s},$$

where these weights are referred as the spatial basis functions (by Kang, et. al., 2010) and others.

Note that, the original random effects γ_s^* are iid, that is, $\gamma_s^* \overset{iid}{\sim} (0, \sigma_\gamma^2)$ irrespective of whether they belong to certain family, we may then write $\widetilde{\gamma}_{sj_s} \overset{iid}{\sim} (0, \sigma_\gamma^2)$ under the s^{th} family. Then the proposed linear equal weights ensure that the random effects for each of the locations belonging to the s^{th} family are treated as equal contributing towards the mean and variance of the responses. This implies that

$$E\left(\frac{1}{\sqrt{n_s}} 1'_{n_s} \widetilde{\gamma}_s\right) = 0 \quad (2.1.8)$$

$$\begin{aligned}\text{Var}\left(\frac{1}{\sqrt{n_s}}1'_{n_s}\widetilde{\gamma}_s\right) &= \text{Var}\left(\frac{1}{\sqrt{n_s}}\sum_{j_s=1}^{n_s}\widetilde{\gamma}_{sj_s}\right)\\ &= \frac{1}{n_s}\left(n_s\sigma_\gamma^2\right) = \sigma_\gamma^2 \qquad (2.1.9)\end{aligned}$$

However, if the $\widetilde{\gamma}_{sj_s}$'s are correlated following a suitable correlation structure, then the combined variance will be affected by the additional pairwise correlations of the random effects. For example, if $\widetilde{\gamma}_{sj_s}$ and $\widetilde{\gamma}_{sj'_s}$ have the correlation $\phi_{j_sj'_s}$, then the contributions of the random effects towards the variation in responses will be affected by these pairwise variable correlations. To be specific, in such a situation, one writes

$$\begin{aligned}\text{var}\left(\frac{1}{\sqrt{n_s}}1'_{n_s}\widetilde{\gamma}_s\right) &= \frac{1}{n_s}\left[\sum_{j_s=1}^{n_s}\text{var}(\widetilde{\gamma}_{sj_s}) + 2\sum_{j_s<j'_s}^{n_s}\text{cov}\left(\widetilde{\gamma}_{sj_s},\widetilde{\gamma}_{sj'_s}\right)\right]\\ &= \frac{1}{n_s}\left[n_s\sigma_\gamma^2 + 2\sum_{j_s<j'_s}^{n_s}\phi_{j_sj'_s}\sigma_\gamma^2\right]\\ &= \sigma_\gamma^2\left[1+\frac{2}{n_s}\sum_{j_s<j'_s}^{n_s}\phi_{j_sj'_s}\right]. \qquad (2.1.10)\end{aligned}$$

However, in practice it may be reasonable to assume constant correlation between pairwise random effects belonging to the same spatial family. Suppose that $\phi_{j_sj'_s} = \phi$ for all $j_s \neq j'_s$. Then (2.1.10) reduces to a simple form

$$\text{var}\left(\frac{1}{\sqrt{n_s}}1'_{n_s}\widetilde{\gamma}_s\right) = \sigma_\gamma^2\left(1+(n_s-1)\phi\right). \qquad (2.1.11)$$

More clearly, by following the model (2.1.7) and using (2.1.11) for the equally correlated pairwise random effect case, for example, we may now write the marginal mean and variance of y_s as

$$E(Y_s) = \mu_s = x_s'\beta, \tag{2.1.12}$$

and

$$\text{var}(Y_s) = \begin{cases} \sigma_\gamma^2 + \sigma_\epsilon^2 & \text{for } \widetilde{\gamma}_{sj_s} \overset{iid}{\sim} (0, \sigma_\gamma^2) \\ \sigma_\gamma^2(1 + (n_s - 1)\phi) + \sigma_\epsilon^2 & \text{for } \widetilde{\gamma}_{sj_s} \sim (0, \sigma_\gamma^2), \ \text{corr}(\widetilde{\gamma}_{sj_s}, \widetilde{\gamma}_{sj_s'}) = \phi \end{cases} \tag{2.1.13}$$

2.2 Correlation Model for Pairwise Responses

Note from (2.1.7) that the response y_s collected from the s^{th} spatial location is influenced by the random effects of a family of neighboring locations denoted by f_s. We now consider another response y_r collected from the r^{th} ($r \neq s$) location which will also be affected by the random effects of a family of neighboring locations denoted by f_r. Note that, similar to y_s, y_r is generated by the relationship (2.1.7) with n_r as the size of the family f_r. Also, similar to $\widetilde{\gamma}_s = (\widetilde{\gamma}_{s1}, \cdots, \widetilde{\gamma}_{sj_s}, \cdots, \widetilde{\gamma}_{sn_s})'$ under f_s we denote the random effects belonging to the family f_r by $\widetilde{\gamma}_r = (\widetilde{\gamma}_{r1}, \cdots, \widetilde{\gamma}_{rj_r}, \cdots, \widetilde{\gamma}_{rn_r})'$. Further note that depending on the distance between the r^{th} and s^{th} locations, y_r and y_s may be affected by the random effects of some common locations. It is expected that the random effects belonging to both families f_r and f_s corresponding to any two member locations will be correlated. It may also happened that the random effects of any two locations where one belongs to f_r and the other belongs to f_s may also be correlated when their distance $d^*_{j_r j_s}$ for $j_r \in f_r$ but $j_r \notin f_s$ and $j_s \in f_s$ but $j_s \notin f_r$. For convenience of construction of the correlation structure between y_r and y_s, we now define

- n_{rs} = the number of members common to both the families (clusters) at r^{th} and s^{th} locations,
- $\overline{n}_r$ = number of members only from the r^{th} family such that

$$n_r = n_{rs} + \overline{n}_r$$

  It also holds for the s^{th} family, that is,

$$n_s = n_{rs} + \overline{n}_s$$

- $\widetilde{n}_{rs}$ =number of uncommon pairs of locations under f_r and f_s, but within the specified distance causing correlations between random effects of these uncommon locations.

2.2.1 Computation of n_{rs} and $\widetilde{n}_{rs}$: An illustration

For clear visual understanding we display above common and uncommon pairs in the following figures.

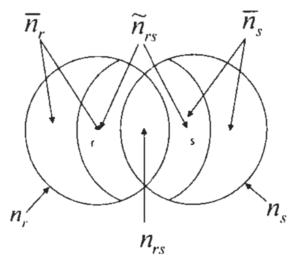

Figure 2.1: Spatial families with n_{rs} common locations and $\widetilde{n}_{rs}$ uncommon pairs

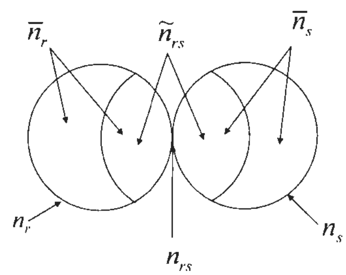

Figure 2.2: Spatial families with single common location

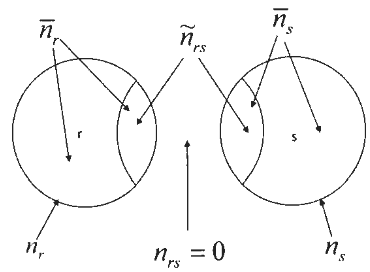

Figure 2.3: Spatial families with no common locations

2.2.2 General spatial correlation design

2.2.2.1 Spatial linear mixed model: A special case in a linear sequence

Suppose that any two random effects corresponding to the locations within distance d^* are correlated. Consider two families f_r and f_s as mentioned earlier. Now to compute the family size, and common members and uncommon but correlated pairs we first give a computational scheme as follows.

2.2.2.2 Pairwise spatial families: A unified computational formula for linear spatial sequence

Let $r(i,j)$ and $s(i,j')$ be two distinct location of events on the linear scale with coordinates (i,j) and (i,j'). Suppose that for a given i, $j' > j$. For this case, for convenience we will use the notation $s > r$. Also let for a given l such that $2l+1 = n_s$, and for $u = -l, \ldots, 0, \cdots, l$; $s + u$ indicates all locations in the s^{th} family f_s. Then the distance limit d^* within which random effects of two locations are correlated can be understood as $(s+l) - (s-l) = d^*$. Now for two spatial locations $r \neq s$ with $n_r = n_s$, we define

$$\begin{aligned} \Delta_{uv} &= (s+v) - (r+u) \\ &= (s-r) + (v-u) \end{aligned}$$

where $r, s = 1, 2, \cdots, S$ and $u, v = -l, \cdots, 0, \cdots, l$. Then the number of members common to both the families (clusters) at r^{th} and s^{th} locations is given by

$$n_{rs} = \begin{cases} 0 & \text{if } \Delta_{uv} > 0 \\ \\ \#\{(s-r) + (v-u) = 0\} & \text{if } \Delta_{uv} \leq 0. \end{cases} \tag{2.2.1}$$

Note if $0 < \Delta_{uv} \leq d^*$ then the number of uncommon pairs $\widetilde{n}_{rs}$ is given by

$$\begin{aligned} \widetilde{n}_{rs} &= \#\{0 < (s-r) + (v-u) \leq d^*\} \\ &- \#(\{0 < (s-r) + (v-u_0) \leq d^*\} \cup \{0 < (s-r) + (v_0-u) \leq d^*\} \\ &\cup \{0 < (s-r) + (v_0-u_0) \leq d^*\}) \\ &\equiv \#\{0 < \Delta_{uv} \leq d^*\} - \#[E_{u_0v} \cup E_{uv_0} \cup E_{u_0v_0}] \end{aligned} \tag{2.2.2}$$

where for chosen u_0 for u and v_0 for v satisfying $(s-r)+(v-u) \leq 0$, and the event E_{uv} in (2.2.2) is defined as

$$E_{uv} = \{0 < (s-r)+(v-u) \leq d^*\}.$$

2.2.2.3 Examples: Based on $d^* = 4$

Example 2.2.1 Linear sequence of two families with three common locations.

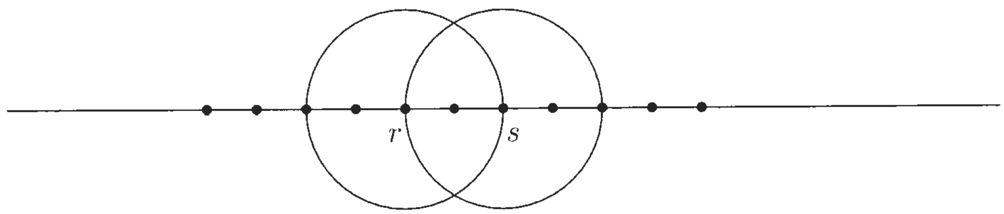

Figure 2.4

In this example, we consider $s - r = 2$ units. For the two families f_r and f_s, it is clear that $n_r = n_s = 5$. Further, for this simple spatial design, it is easy to count the number of common members and uncommon number of pairs of locations. These are given as

$$\begin{aligned}
n_{rs} &= 3 \\
\overline{n}_r &= n_r - n_{rs} = 5-3 = 2 \\
\overline{n}_s &= n_s - n_{rs} = 5-3 = 2 \\
\widetilde{n}_{rs} &= 1
\end{aligned}$$

We now verify that (2.2.1) and (2.2.2) may be applied to obtain the above sizes. To be more specific,

$$\begin{aligned}\Delta_{uv} &= (s-r)+(v-u)\\ &= 2+(v-u)\end{aligned} \qquad (2.2.3)$$

where, $u, v = -l, \cdots, 0, \cdots, l$, with l satisfying $2l+1 = n_r = n_s = 5$. For $l = 2$, Δ_{uv}'s in (2.2.3) are

							E_{u_0v}	E_{uv_0}	$E_{u_0v_0}$
Δ	=	2	+	$(-2+2)$	=	2		×	
	=	2	+	$(-2+1)$	=	1		×	
	=	2	+	$(-2-0)$	=	0			
	=	2	+	$(-2-1)$	=	-1			
	=	2	+	$(-2-2)$	=	-2			
	=	2	+	$(-1+2)$	=	3		×	
	=	2	+	$(-1+1)$	=	2		×	
	=	2	+	$(-1-0)$	=	1	*	×	+
	=	2	+	$(-1-1)$	=	0			
	=	2	+	$(-1-2)$	=	-1			
	=	2	+	$(0+2)$	=	4		×	
	=	2	+	$(0+1)$	=	3		×	
	=	2	+	$(0-0)$	=	2	*	×	+
	=	2	+	$(0-1)$	=	1	*	×	+
	=	2	+	$(0-2)$	=	0			
	=	2	+	$(1+2)$	=	5			
	=	2	+	$(1+1)$	=	4			
	=	2	+	$(1-0)$	=	3	*		
	=	2	+	$(1-1)$	=	2	*		
	=	2	+	$(1-2)$	=	1	*		
	=	2	+	$(2+2)$	=	6			
	=	2	+	$(2+1)$	=	5			
	=	2	+	$(2-0)$	=	4	*		
	=	2	+	$(2-1)$	=	3	*		
	=	2	+	$(2-2)$	=	2	*		

Note that there are 6 cases and among these cases there are 3 cases with $\Delta_{uv} = 0$. That is,

$$\#\{\Delta_{uv} = 0\} = 3.$$

Hence by (2.2.1) $n_{rs} = 3$.

Next we select u_0 and v_0 satisfying $\Delta_{u_0v_0} = 2 + (v_0 - u_0) \leq 0$. The selected values are

$$u_0 = 0, 1, 2 \text{ and } v_0 = -2, -1, 0.$$

For $d^* = 4$, and for all possible values of u and v we have

$$\#\{0 < \Delta_{uv} \leq d^*\} = 16.$$

When $u = u_0 \equiv (0, 1, 2)$ and v is general, that is, $v \equiv (-2, -1, 0, 1, 2)$, we count the number of Δ_{uv} satisfying $0 < \Delta_{uv} \leq d^*$ and obtain $\#E_{u_0v} = 9$. Similarly $\#E_{uv_0} = 9$ and $\#E_{u_0v_0} = 3$

Hence $\widetilde{n}_{rs} = 16 - 15 = 1$

Example 2.2.2 Linear sequence of two families with one common location

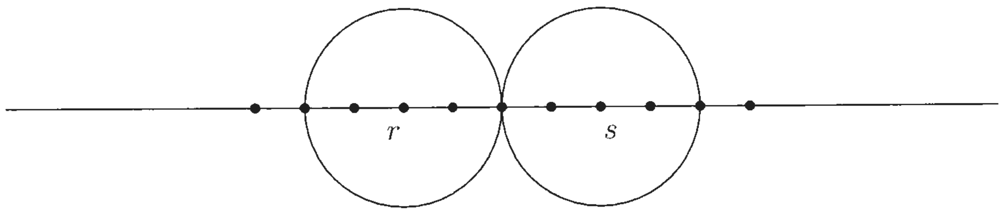

Figure 2.5

Consider $s - r = 4$ units. Similar to example 1, in this case we have

$$\begin{aligned}
n_{rs} &= 1 \\
\overline{n}_r &= n_r - n_{rs} = 5 - 1 = 4 \\
\overline{n}_s &= n_s - n_{rs} = 5 - 1 = 4 \\
\widetilde{n}_{rs} &= 6
\end{aligned}$$

Example 2.2.3 Linear sequence of two families with no common locations but $\widetilde{n}_{rs} > 0$.

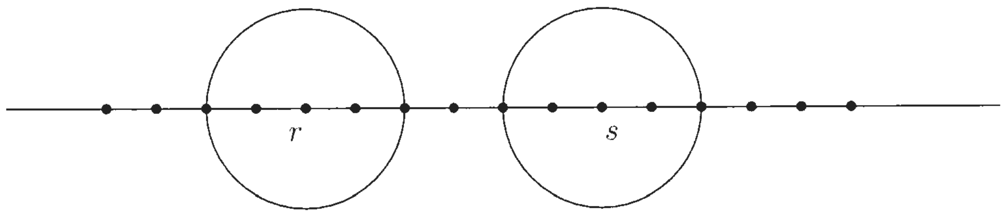

Figure 2.6

Here $s - r = 6$ units. We then have

$$\begin{aligned} n_{rs} &= 0 \\ \overline{n}_r &= n_r - n_{rs} = 5 - 0 = 5 \\ \overline{n}_s &= n_s - n_{rs} = 5 - 0 = 5 \\ \widetilde{n}_{rs} &= 6 \end{aligned}$$

Example 2.2.4 Linear sequence of two families with no correlation ($\widetilde{n}_{rs} = 0$)

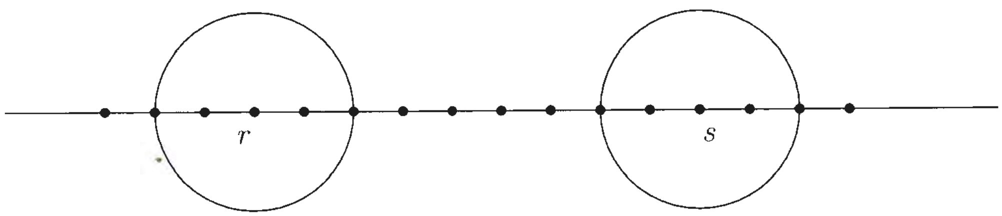

Figure 2.7

Consider $s - r = 9$ units. We then have the following sizes

$$\begin{aligned} n_{rs} &= 0 \\ \overline{n}_r &= n_r - n_{rs} = 5 - 0 = 5 \\ \overline{n}_s &= n_s - n_{rs} = 5 - 0 = 5 \\ \widetilde{n}_{rs} &= 0 \end{aligned}$$

2.3 Marginal and Correlation Properties of the Proposed Spatial Model

Recall from (2.1.7), that the s^{th} response follows the model

$$y_s = x_s'\beta + \frac{1}{\sqrt{n_s}} 1_{n_s}' \widetilde{\gamma}_s + \epsilon_s, \quad \text{for } s = 1, \cdots, S, \tag{2.3.1}$$

where β is the regression effects of x_s on y_s for all $s = 1, \cdots, S$ and $\widetilde{\gamma}_s = (\widetilde{\gamma}_{s1}, \cdots, \widetilde{\gamma}_{sn_s})'$ with $j_s(= 1, \cdots, n_s)$, $\widetilde{\gamma}_{sj_s} = \gamma_{sk}$ for any $k \in f_s$. Recall from (2.1.4) that γ_{sk} is the k^{th} random effect in the s^{th} family, that is, $\gamma_{sk} = \gamma_k^*$ for $k \in f_s$. Because by (2.1.3a), $\gamma_k^* \sim (0, \sigma_\gamma^2)$ for any $k = 1, 2, \cdots, S$. It then follows that for $j_s = 1, \cdots, n_s$ and for any $k(= 1, \cdots, S) \in f_s$

$$\widetilde{\gamma}_{sj_s} = \gamma_{sk} \sim (0, \sigma_\gamma^2) \tag{2.3.2}$$

Now for $k \neq l$ consider

$$\gamma_{sk} = \gamma_k^* \text{ and } \gamma_{sl} = \gamma_l^* \text{ for } k, l \in f_s. \tag{2.3.3}$$

Because by (2.1.3b), $\text{corr}(\gamma_k^*, \gamma_l^*) = \delta_{kl}\phi_{kl}^*$, for $k \equiv j_s \in f_s$ and $l \equiv j_s' \in f_s$, it then follows that

$$\text{corr}(\widetilde{\gamma}_{sj_s}, \widetilde{\gamma}_{sj_s'}) = \text{corr}(\gamma_{sk}, \gamma_{sl}) = \text{corr}(\gamma_k^*, \gamma_l^*) = \delta_{kl}\phi_{kl}^*. \tag{2.3.4}$$

Because $\delta_{kl} = 1$ as $k, l \in f_s$, by using $\phi_{kl}^* = \phi_{kl}(s)$, we write

$$\text{corr}(\widetilde{\gamma}_{sj_s}, \widetilde{\gamma}_{sj_s'}) = \phi_{kl}(s), \tag{2.3.5}$$

where these parameters σ_γ^2 in (2.3.2) and $\phi_{kl}(s)$ in (2.3.5) are determined by the properties of the random effects $\gamma_1^*, \cdots, \gamma_S^*$ associated to all s locations, and following the specification (2.3.3), namely $\gamma_{sk} = \gamma_k^*$ for $k \in f_s$. Also for the model error in

(2.3.1), it has been assumed that

$$\epsilon_s \overset{iid}{\sim} (0, \sigma_\epsilon^2). \tag{2.3.6}$$

Furthermore ϵ_s and γ_{sk} (or γ_k^*) are assumed to be independent

2.3.1 Marginal Properties

By using the model (2.3.1)-(2.3.6), we now write the mean and variance of y_s as in the following lemma.

Lemma 2.3.1 The mean, $E(Y_s)$ and the variance, $\text{var}(Y_s)$ are given by

$$E(Y_s) = \mu_s = x_s'\beta, \tag{2.3.7}$$

$$\begin{aligned}
\text{var}(Y_s) &= \frac{1}{n_s}\text{var}\left(\sum_{j_s=1}^{n_s} \widetilde{\gamma}_{sj_s}\right) + \text{var}(\epsilon_s) \\
&= \frac{1}{n_s}\left[\sum_{j_s=1}^{n_s} \text{var}\left(\widetilde{\gamma}_{sj_s}\right) + 2\sum_{j_s<j_s'}^{n_s} \text{cov}\left(\widetilde{\gamma}_{sj_s}, \widetilde{\gamma}_{sj_s'}\right)\right] + \sigma_\epsilon^2 \\
&= \frac{1}{n_s}\left[n_s\sigma_\gamma^2 + 2\sum_{j_s<j_s'}^{n_s} \phi_{j_sj_s'}(s)\sigma_\gamma^2\right] + \sigma_\epsilon^2 \\
&= \sigma_\gamma^2\left[1 + \frac{2}{n_s}\sum_{j_s<j_s'}^{n_s} \phi_{j_sj_s'}(s)\right] + \sigma_\epsilon^2 \\
&= \sigma_{ss} \quad (\text{say}).
\end{aligned} \tag{2.3.8}$$

Note that for a special case when $\phi_{j_s j'_s}(s) = \phi$ for all $j_s \neq j'_s$, (2.3.8) reduces to a simpler form

$$\sigma_{ss} = \sigma_\gamma^2 [1 + (n_s - 1)\phi] + \sigma_\epsilon^2 \tag{2.3.9}$$

which further simplifies to

$$\sigma_{ss} = \sigma_\gamma^2 + \sigma_\epsilon^2 = \sigma^2 \text{ (say)} \tag{2.3.10}$$

when random effects are independent, that is $\phi_{j_s j'_s}(s) = \phi = 0$.

2.3.2 Correlation Properties

Now for any two spatial locations r and s such that $(r \neq s)$, let the responses y_r and y_s be generated by (2.3.1). Recall that y_r is influenced by the n_r number of neighboring locations but they belong to the family f_r. Similarly y_s is influenced by the n_s number of neighboring locations but they belonging to the family f_s. Also recall that depending on the distance between the r^{th} and s^{th} locations, y_r and y_s may be affected by the random effects of some common locations and uncommon pairs of locations. Thus the covariance, $\text{cov}(Y_r, Y_s)$ between two responses at the r^{th} and s^{th} locations may be computed by using the following lemma.

Lemma 2.3.2 The covariance between two responses y_r and y_s at a given two spatial locations r and s $(r \neq s)$ is given by

$$\begin{aligned}
\text{cov}\,(Y_r, Y_s) &= \frac{1}{\sqrt{n_r n_s}} \text{cov}\left(\sum_{j_r=1}^{n_r} \widetilde{\gamma}_{rj_r}, \sum_{j_s=1}^{n_s} \widetilde{\gamma}_{sj_s} \right) \\
&= \frac{1}{\sqrt{n_r n_s}} \sum_{j_r=1}^{n_r} \sum_{j_s=1}^{n_s} \text{cov}\,(\widetilde{\gamma}_{rj_r}, \widetilde{\gamma}_{sj_s}) \\
&= \frac{1}{\sqrt{n_r n_s}} \sum_{j,} \sum_{k\ \in f_r \cup f_s} \delta_{jk} \phi^*_{jk} \sigma^2_\gamma \\
&= \sigma_{rs} \ \ (\text{say}),
\end{aligned} \tag{2.3.11}$$

with $\delta_{jk} = 1$ and $\phi^*_{jk} = 1$ for $j = k$. More specifically

$$\begin{aligned}
\sigma_{rs} &= \frac{1}{\sqrt{n_r n_s}} \left(\sum_{j_r, j'_r \in G_1} \phi^*_{j_r j'_r} \sigma^2_\gamma + \sum_{j_r \neq j'_r \in G_2} \phi^*_{j_r j'_r} \sigma^2_\gamma \right. \\
&\left. + \sum_{j_s \neq j'_s \in G_3} \phi^*_{j_s j'_s} \sigma^2_\gamma + \sum_{j_r \in \overline{f}_s, j_s \in G_4} \delta_{j_r j_s} \phi^*_{j_r j_s} \sigma^2_\gamma \right)
\end{aligned} \tag{2.3.12}$$

By identifying the four groups G in (2.3.12) as

$$\begin{aligned}
j_r, j'_r \in f_r \cap f_s &\equiv G_1 \\
j_r \in f_r \cap f_s,\ j'_r \in f_r \cap \overline{f}_s &\equiv G_2 \\
j_s \in f_r \cap f_s,\ j'_s \in f_s \cap \overline{f}_r &\equiv G_3 \\
j_r \in \overline{f}_s,\ \ j_s \in \overline{f}_r &\equiv G_4
\end{aligned}$$

and denoting the correlation in the l^{th} $(l = 1, 2, 3, 4)$ group as

$$\phi^{(l)}_{jk} \ \text{ for } \ j, k \in G_l, \tag{2.3.13}$$

we reexpress the covariance in (2.3.12) as

$$\sigma_{rs} = \frac{\sigma_\gamma^2}{\sqrt{n_r n_s}} \Bigg(\sum_{j,k \in G_1} \phi_{jk}^{(1)} + \sum_{j,k \in G_2} \phi_{jk}^{(2)} + \sum_{j,k \in G_3} \phi_{jk}^{(3)} + \sum_{j,k \in G_4} \delta_{jk} \phi_{jk}^{(4)} \Bigg) \quad (2.3.14)$$

2.3.2.1 An equi-correlation case within a distance d^*

Suppose that any two random effects within a distance d^* share a common family effect. In such a familial setup it is appropriate to assume that pairwise random effects within the family will be equally correlated. Let ϕ denote this correlation, In this case, it follows from Figure 2.1 in Section 2.2.1 that

1. $j, k \in G_1$ provide variance and the covariance from n_{rs} common members for the r^{th} and s^{th} families of locations.

2. For $j \neq k$, $j, k \in G_2$ the second term in (2.3.14) provides the total covariance among $\bar{n}_r$ members belonging to $\overline{f}_s \cap f_r$ and n_{rs} members belonging to $f_r \cap f_s$.

3. Similarly for $j \neq k$, $j, k \in G_3$ we have covariances between $\bar{n}_s$ members belonging to $\overline{f}_r \cap f_s$ and n_{rs} members belonging to $f_r \cap f_s$.

4. Finally, for $j, k \in G_4$, one obtains covariances among the members in $\overline{f}_r$ and $\overline{f}_s$ respectively.

Combining (1) to (4) we now write the specific formula for σ_{rs} in (2.3.14) as

$$\begin{aligned}\sigma_{rs} &= \frac{1}{\sqrt{n_r n_s}}\left[n_{rs}\sigma_\gamma^2 + \left(n_{rs}(n_{rs}-1) + n_{rs}\overline{n}_r + n_{rs}\overline{n}_s + \widetilde{n}_{rs}\right)\phi\sigma_\gamma^2\right] \\ &= \frac{1}{\sqrt{n_r n_s}}\left[n_{rs} + \left(n_{rs}(n_{rs}-1) + n_{rs}\overline{n}_r + n_{rs}\overline{n}_s + \widetilde{n}_{rs}\right)\phi\right]\sigma_\gamma^2. \qquad (2.3.15)\end{aligned}$$

Now let Σ be the covariance matrix of the model (2.3.1) so that $\Sigma = (\sigma_{rs})$, where σ_{rs} are defined as.

$$\sigma_{rs} = \begin{cases} \left[1 + (n_s - 1)\phi\right]\sigma_\gamma^2 + \sigma_\epsilon^2 & \text{if } r = s, \\ \\ \frac{1}{\sqrt{n_r n_s}}\left\{n_{rs}\left[1 + (n_{rs} - 1 + \overline{n}_r + \overline{n}_s)\phi\right] + \widetilde{n}_{rs}\phi\right\}\sigma_\gamma^2 & \text{otherwise.} \end{cases} \qquad (2.3.16)$$

In some cases it may happen that a family of locations may be independent from another family of locations. In this type of special situation, it is only necessary to compute the familial correlations of the responses under a given family. These correlations can be computed as a special case of Lemma 2.3.2

Lemma 2.3.3 Consider two responses y_{sj_s} and $y_{sj'_s}$ within the s^{th} family. For obtaining their correlations from two families based on the general results of Lemma 2.3.2, one may suppress the family notation and denote these responses as y_{j_s} and

$y_{j'_s}$. Now the covariance between these two responses y_{j_s} and $y_{j'_s}$ is given by

$$\text{cov}\left(y_{j_s}, y_{j'_s}\right) = \sigma_{j_s j'_s} = \sigma^2_\gamma \left[1 + \frac{2}{n_s}\sum_{l_s<l'_s}^{n_s} \phi_{l_s l'_s}(s)\right]. \tag{2.3.17}$$

where $\phi_{l_s l'_s}(s)$ is the correlation between two random effects in (2.3.5).

Proof: Because,

$$\begin{aligned} y_{j_s} &= x'_{j_s}\beta + \frac{1}{\sqrt{n_{j_s}}} 1'_{n_{j_s}}\gamma_{j_s} + \epsilon_{j_s}, \quad j_s \in f_s \\ y_{j'_s} &= x'_{j'_s}\beta + \frac{1}{\sqrt{n_{j'_s}}} 1'_{n_{j'_s}}\gamma_{j'_s} + \epsilon_{j'_s}, \quad j'_s \in f_s. \end{aligned}$$

and because $1'_{n_{j_s}}\gamma_{j_s} = 1'_{n_{j'_s}}\gamma_{j'_s}$, one obtains the covariance between y_{j_s} and $y_{j'_s}$ as in the lemma by comparing γ_{j_s} with γ_{rj_r} and $\gamma_{j'_s}$ with γ_{sj_s} of Lemma 2.3.2 such that now $f_r \cap f_s$ reduces to f_s. Thus we simply use the first term $\left(\sum_{l_s, l'_s \in G_1} \phi^{(1)}_{l_s l'_s}\right)$ from (2.3.14) and write the $\text{cov}\left(y_{j_s}, y_{j'_s}\right)$ as

$$\begin{aligned} \sigma_{j_s j'_s} &= \frac{1}{\sqrt{n_{j_s} n_{j'_s}}} \sum_{l_s, l'_s \in f_s} \phi^*_{l_s l'_s}\sigma^2_\gamma \\ &= \frac{\sigma^2_\gamma}{\sqrt{n_{j_s} n_{j'_s}}} \sum_{j,k \in f_s} \phi^{(1)}_{jk}. \end{aligned} \tag{2.3.18}$$

Hence, for $n_{j_s} = n_{j'_s} = n_s$, (2.3.18) gives

$$\begin{aligned} \sigma_{j_s j'_s} &= \frac{\sigma_\gamma^2}{n_s}\left[\sum_{l_s = l'_s}^{n_s} \phi_{l_s l'_s}(s) + 2\sum_{l_s < l'_s}^{n_s} \phi_{l_s l'_s}(s)\right] \\ &= \frac{\sigma_\gamma^2}{n_s}\left[n_s + 2\sum_{l_s < l'_s}^{n_s} \phi_{l_s l'_s}(s)\right] \\ &= \sigma_\gamma^2\left[1 + \frac{2}{n_s}\sum_{l_s < l'_s}^{n_s} \phi_{l_s l'_s}(s)\right], \end{aligned} \tag{2.3.19}$$

which is the same as in the lemma.

Chapter 3

Inference in Spatial Linear Mixed Model

In the last chapter, more specifically in equation (2.3.1) we have used a linear model for the response y_s as a function of location specified fixed effects as well as familial random effects, where the s^{th} family contains n_s neighboring locations each associated with an unobservable random effect. Note that correlation between any two responses y_r and y_s for $r \neq s$ is also modeled through Lemma 2.3.1. Now for the inferences about the effects β of fixed covariates as well as random effects, it is convenient to write the combined model for all responses $y_1, \cdots, y_r \cdots, y_s, \cdots, y_S$ in a matrix form, which we provide as follows.

3.1 Model in Matrix Notation and Estimation

For convenience, we re-write the spatial model (2.3.1) in matrix notation as follows:

$$Y = X\beta + U^*\widetilde{G} + \epsilon, \tag{3.1.1}$$

where $Y = (y_1, \cdots, y_S)$ is the $S \times 1$ vector of response variables, $X = (x_1, \cdots, x_S)'$ is the $S \times p$ covariate matrix, $\beta = (\beta_1, \cdots, \beta_p)'$ is the corresponding $p \times 1$ regression parameter vector, and $\epsilon = (\epsilon_1, \cdots, \epsilon_S)$ is $S \times 1$ error vector with zero mean and $\text{cov}(\epsilon) = \sigma^2 I_S$. Furthermore, in (3.1.1), for $N = \sum_{s=1}^{S} n_s$, $U^* = \bigoplus_{s=1}^{S} \frac{1}{\sqrt{n_s}} 1'_{n_s} \ : \ S \times N$, is a block diagonal matrix with its $s^{\text{th}}(s = 1, \cdots, S)$ diagonal block as the $1 \times n_s$ vector with each elements as $\frac{1}{\sqrt{n_s}}$, and $\widetilde{G} = (\widetilde{\gamma}'_1, \cdots, \widetilde{\gamma}'_s \cdots, \widetilde{\gamma}'_S)'$ is an $N \times 1$ vector of familial random variables, where, it is likely that $\widetilde{\gamma}'_s$ and $\widetilde{\gamma}'_{s\pm1}$, for example, have some overlapping random effects. We now express the mean vector and covariance matrix of Y as

$$\mu(\beta) = E(Y) = (\mu_1(\beta), \cdots, \mu_S(\beta))', \tag{3.1.2}$$

and

$$\Sigma = \text{Cov}(Y) = \left(\sigma_{rs}(\sigma_\gamma^2, \sigma_\epsilon^2, \phi_{jk})\right), \quad \text{with} \quad j, k \in [f_r \cup f_s], \tag{3.1.3}$$

where $\mu_s(\beta) = E(Y_s)$ and σ_{ss} are given by (2.3.7) and (2.3.8) respectively, whereas for $r \neq s$, σ_{rs} is given by (2.3.14). Note that $\mu_s(\beta) = E(Y_s)$ is a function of the

β parameter vector, and variances σ_{ss} and the covariances σ_{rs} are functions of the scale parameters σ_γ^2 and σ_ϵ^2, and the correlation parameters ϕ_{jk}. Note that ϕ_{jk} for $j, k \in [f_r \cup f_s]$ have links with the original ϕ_{jk}^* for $j, k \in \mathcal{S}$, the complete space.

3.2 Generalized Least Squares (GLS) Estimation

3.2.1 GLS Estimation of Regression Effect β

It is convenient to write an estimating equation for the regression effects β under the general model, that is, when random effects follow a familial correlation structure. The estimation for β when random effects are independent becomes a special case.

Because the β parameter is involved only in the mean function, we can use the standard generalized least squares (GLS) (Amemiya 1985) result to estimate β by solving

$$\frac{\partial \mu'(\beta)}{\partial \beta} \Sigma^{-1}(y - \mu(\beta)) \quad = \quad 0, \tag{3.2.1}$$

where by (3.1.2), $\mu(\beta) = (\mu_1(\beta), \cdots, \mu_S(\beta))'$ and $\mu_s(\beta) = x_s'\beta$ with $\frac{\partial \mu_s(\beta)}{\partial \beta} = x_s$ and by (3.1.3), $\Sigma = (\sigma_{rs}(\sigma_\gamma^2, \sigma_\epsilon^2, \phi_{jk}))$.

Note that the covariance matrix Σ does not involve β, and for known Σ, the solution for β from (3.2.1) is straightforward under the present linear mixed model. By (3.2.1) the generalized least squares (GLS) estimator of β has the formula given by

$$\hat{\beta}_{GLS} = \left[X'\Sigma^{-1}X\right]^{-1}\left[X'\Sigma^{-1}Y\right]. \tag{3.2.2}$$

where Σ is given by (3.1.3). Note that $\hat{\beta}_{GLS}$ in (3.2.2) requires Σ to be known, that is σ_γ^2, σ_ϵ^2 and all ϕ_{jk} for $j, k \in [f_r \cup f_s]$ need to be estimated. However, as these scale and correlation parameters are unknown in practice, we provide a consistent estimation approach for these scale parameters in Section **3.2.2**. Note that the construction of the moment estimating equations will depend on the familial correlation structure for the random effects. This will be done under two scenarios: first, assuming that the random effects are independent and then by using a familial correlation structure for random effects.

Chapter 3

Inference in Spatial Linear Mixed Model

In the last chapter, more specifically in equation (2.3.1) we have used a linear model for the response y_s as a function of location specified fixed effects as well as familial random effects, where the s^{th} family contains n_s neighboring locations each associated with an unobservable random effect. Note that correlation between any two responses y_r and y_s for $r \neq s$ is also modeled through Lemma 2.3.1. Now for the inferences about the effects β of fixed covariates as well as random effects, it is convenient to write the combined model for all responses $y_1, \cdots, y_r \cdots, y_s, \cdots, y_S$ in a matrix form, which we provide as follows.

that is,

$$\begin{aligned} E\left(\hat{\beta}_{GLS}\right) &= E\left(\left[X'\Sigma^{-1}X\right]^{-1}\left[X'\Sigma^{-1}y\right]\right) \\ &= \left[X'\Sigma^{-1}X\right]^{-1}\left[X'\Sigma^{-1}E(Y)\right] \\ &= \left[X'\Sigma^{-1}X\right]^{-1}\left[X'\Sigma^{-1}X\beta\right] \\ &= \beta. \end{aligned} \tag{3.2.3}$$

Furthermore it follows that

$$\begin{aligned} V\left(\hat{\beta}_{GLS}\right) &= \left[X'\Sigma^{-1}X\right]^{-1} X'\Sigma^{-1}V(Y)\Sigma^{-1}X\left[X'\Sigma^{-1}X\right]^{-1} \\ &= \left[X'\Sigma^{-1}X\right]^{-1} X'\Sigma^{-1}\Sigma\Sigma^{-1}X\left[X'\Sigma^{-1}X\right]^{-1} \\ &= \left[X'\Sigma^{-1}X\right]^{-1}\left[X'\Sigma^{-1}X\right]\left[X'\Sigma^{-1}X\right]^{-1} \\ &= \left[X'\Sigma^{-1}X\right]^{-1}, \end{aligned} \tag{3.2.4}$$

which may be estimated directly by estimate the Σ consistently, which we discuss in the next section.

3.2.2 Moment Estimation of Scale and Correlation Parameters

3.2.2.1 When Random Effects are Independent

When random effects are independent, the covariance matrix Σ in (3.1.3) has the form

$$\Sigma = (\sigma_{rs}) \text{ with } \sigma_{rs} = \text{cov}(Y_r, Y_s) = \begin{cases} \sigma^2 & \text{if } r = s \\ \frac{n_{rs}}{\sqrt{n_r n_s}} R_{\sigma_\gamma} \sigma^2 & \text{otherwise,} \end{cases} \tag{3.2.5}$$

where $R_{\sigma_\gamma} = \frac{\sigma_\gamma^2}{\sigma^2}$. This is because for $r = s$ it follows from (2.3.8) that

$$\begin{aligned} \sigma_{ss} &= \text{var}(Y_s) \\ &= \sigma_\gamma^2 \left[1 + \frac{2}{n_s} \sum_{j_s < j_s'}^{n_s} \phi_{j_s j_s'}(s) \right] + \sigma_\epsilon^2. \end{aligned}$$

Note that, $\phi_{j_s j_s'}(s)$ is the correlation between the random effects $\tilde{\gamma}_{sj_s}$ and $\tilde{\gamma}_{sj_s'}$ belonging to the s^{th} family. Thus, when it is assumed that the random effects are independent, one writes $\phi_{j_s j_s'}(s) = 0$. That is,

$$\begin{aligned} \sigma_{ss} &= \text{var}(Y_s) \\ &= \sigma_\gamma^2 + \sigma_\epsilon^2 \\ &= \sigma^2 \end{aligned}$$

as in (3.2.5).

Next, for $r \neq s$ even though the random effects are independent, σ_{rs} the covariance between y_r and y_s will not be zero. This is because in (2.3.14), all groups except G_1 contain correlation of pairwise random effects. These pairwise correlations in all groups except G_1, are zero when random effects are independent. However, under G_1, one writes

$$\begin{aligned} \sum_{j,k \in G_1} \phi_{jk}^{(1)} &= \sum_{j=k \in [f_r \cap f_s]} \phi_{jk}^{(1)} + \sum_{j \neq k \in [f_r \cap f_s]} \phi_{jk}^{(1)} \\ &= \sum_{j=1}^{n_{rs}} \phi_{jj}^{*} + 0 \\ &= n_{rs} \quad \text{as} \quad \phi_{jj} = 1, \end{aligned}$$

yielding,

$$\sigma_{rs} = \frac{n_{rs}\sigma_{\gamma}^{2}}{\sqrt{n_r n_s}}.$$

Note that the covariance structure (3.2.5) produces the correlations between any two spatial responses y_r and y_s as:

$$\text{corr}\,(Y_r, Y_s) = \begin{cases} 1 & \text{if } r = s \\ \dfrac{n_{rs}}{\sqrt{n_r n_s}} R_{\sigma_\gamma} & \text{otherwise.} \end{cases} \tag{3.2.6}$$

Now by exploiting the covariance structure (3.2.5) we develop moment estimating equations for the scale parameters σ^2 and R_{σ_γ} as in the following section.

3.2.2.2 Estimation of Scale Parameters

The moment estimates of the scale parameters are given in the following lemma.

Lemma 3.2.1 By using the sample variance and lag one correlation we obtain the estimators for σ^2 and R_{σ_γ} as:

$$\hat{\sigma}^2 = \frac{1}{S}\sum_{s=1}^{S}(y_s - \mu_s)^2, \tag{3.2.7}$$

and

$$\hat{R}_{\sigma_\gamma} = \frac{r_1(S-1)}{\sum_{s=1}^{S-1}\frac{n_{s,s+1}}{\sqrt{n_s n_{s+1}}}}, \tag{3.2.8}$$

where, r_1 is the sample lag one correlation.

Proof: Because $E(Y_s) = \mu_s$, it is clear that

$$\begin{aligned} E\left(\frac{1}{S}\sum_{s=1}^{S}(y_s - \mu_s)^2\right) &= \frac{1}{S}\sum_{s=1}^{S} E\left(y_s - \mu_s\right)^2 \\ &= \frac{1}{S}\sum_{s=1}^{S}\text{var}(y_s) \\ &= \sigma^2 \end{aligned}$$

by (3.2.5). Consequently, we obtain the moment estimator of σ^2 as in (3.2.7), where β is assumed to be known.

Next, for known β, the sample lag one correlation of the model is given by

$$r_1 = \frac{\sum_{s=1}^{S-1}(y_s - \mu_s)(y_{s+1} - \mu_{s+1})/(S-1)}{\sum_{s=1}^{S}(y_s - \mu_s)^2/S}. \quad (3.2.9)$$

By using the first order approximation, one may obtain

$$\begin{aligned} E(r_1) &\cong \frac{E\left(\sum_{s=1}^{S-1}(y_s - \mu_s)(y_{s+1} - \mu_{s+1})/(S-1)\right)}{E\left(\sum_{s=1}^{S}(y_s - \mu_s)^2/S\right)} \\ &= \frac{\frac{1}{S-1}\sum_{s=1}^{S-1}\frac{n_{s,s+1}}{\sqrt{n_s n_{s+1}}}R_{\sigma_\gamma}\sigma^2}{S\sigma^2/S} \quad \text{by (3.2.5)} \\ &= \frac{R_{\sigma_\gamma}}{S-1}\sum_{s=1}^{S-1}\frac{n_{s,s+1}}{\sqrt{n_s n_{s+1}}}. \quad (3.2.10) \end{aligned}$$

Consequently, the moment estimating equation for R_{σ_γ} has the form

$$r_1 = \frac{R_{\sigma_\gamma}}{S-1}\sum_{s=1}^{S-1}\frac{n_{s,s+1}}{\sqrt{n_s n_{s+1}}}, \quad (3.2.11)$$

yielding the moment estimator for R_{σ_γ} as in (3.2.8).

Note that, when needed, the scale parameters σ_γ^2 and σ_ϵ^2 may be estimated as follows by using their functional relationship with σ^2 and R_{σ_γ}:

$$\hat{\sigma}_\gamma^2 = \frac{r_1(S-1)}{\sum_{s=1}^{S-1} \frac{n_{s,s+1}}{\sqrt{n_s n_{s+1}}}} \hat{\sigma}^2, \tag{3.2.12}$$

and

$$\hat{\sigma}_\epsilon^2 = \hat{\sigma}^2 - \hat{\sigma}_\gamma^2. \tag{3.2.13}$$

Thus, to obtain $\hat{\beta}_{GLS}$ and moment estimators for the scale parameters we may use the following steps:

Step 1: For a suitable initial values of σ_γ^2 and σ_ϵ^2, estimate β by using (3.2.2).

Step 2: Using β estimate from Step 1, we compute $\hat{\sigma}^2$ and $\hat{R}_{\sigma_\gamma}$ by (3.2.7) and (3.2.8) respectively. They provide estimates of σ_γ^2 and σ_ϵ^2 as in (3.2.12) and (3.2.13).

The moment estimates for the scale parameters from Step 2 are then used in Step 1 to obtain an improved estimate of β. This constitutes a cycle of iterations which continues until convergence. Note that because moment estimators considered have converge to their respective expectations, the convergence of the iterations is assumed by their moment property.

3.2.2.3 When Random Effects follow a Familial Correlation Structure: An Equi-correlation (EQC)/Exchangeable Model

Recall that in general under the whole spatial region

$$\gamma_s^* \sim (0, \sigma_\gamma^2), \qquad s = 1, \cdots, S \tag{3.2.14a}$$

and

$$\text{corr}(\gamma_r^*, \gamma_s^*) = \delta_{rs}\phi_{rs}^*, \qquad r, s = 1, \cdots, S. \tag{3.2.14b}$$

We now assume that any two random effects γ_r^* and γ_s^* corresponding to the r^{th} and s^{th} locations when $r, s \in \mathcal{S}$, have the same correlation as $\phi^* = \phi$ when $\delta_{rs} = 1$, where

$$\delta_{rs} = \begin{cases} 1 \text{ if } d_{rs}^* \leq d^* \text{ for } r, s = 1, \cdots, S \\ 0 \text{ otherwise,} \end{cases}$$

with d^* is the pre specified distance chosen by the user.

It then follows that all random effects $\widetilde{\gamma}_{s1}, \cdots, \widetilde{\gamma}_{sj_s}, \cdots, \widetilde{\gamma}_{sn_s}$ belonging to the same (s^{th}) family have the correlation structure as

$$\text{corr}(\widetilde{\gamma}_{sj_s}, \widetilde{\gamma}_{sj'_s}) = \begin{cases} 1 & \text{for } j_s = j'_s \\ \phi & \text{for } j_s \neq j'_s, \end{cases} \tag{3.2.14c}$$

where $\widetilde{\gamma}_{sj_s}$ is the j_s^{th} component of $\widetilde{\gamma}_s = (\widetilde{\gamma}_{s1}, \cdots, \widetilde{\gamma}_{sj_s}, \cdots, \widetilde{\gamma}_{sn_s})'$, as in (2.1.5), the vector of random effects for locations under the s^{th} family/cluster.

3.2.2.4 Estimation of Scale and Correlation Parameters

Note that, when the random effects are exchangeable, the basic properties of the model (2.3.1) [see also (2.1.7)] such as, the mean, variance and the covariance are given by (2.3.7),(2.3.9) and (2.3.15) respectively.

One may then attempt to write appropriate ordinary moment equations in order to obtain method of moments (MM) estimators for the scale parameters σ_γ^2, σ_ϵ^2 and correlation parameter ϕ. To be specific, following a time series approach (Box and Jenkins 1970), one estimates these scale parameters by using three estimating equations that are constructed based on three basic statistics given by

$$W_1 = \frac{1}{S}\sum_{s=1}^{S}(y_s - \mu_s)^2; \quad \text{lag 0 based,} \tag{3.2.15}$$

$$W_2 = \frac{\sum_{s=1}^{S-1}(y_s - \mu_s)(y_{s+1} - \mu_{s+1})/(S-1)}{\sum_{s=1}^{S}(y_s - \mu_s)^2/S}; \quad \text{lag 1 based,} \tag{3.2.16}$$

$$W_3 = \frac{\sum_{s=1}^{S-2}(y_s - \mu_s)(y_{s+2} - \mu_{s+2})/(S-2)}{\sum_{s=1}^{S}(y_s - \mu_s)^2/S}; \quad \text{lag 2 based,} \tag{3.2.17}$$

Let $W = (W_1, W_2, W_3)'$ be the 3 - dimensional vector of these statistics and $\lambda = (\lambda_1, \lambda_2, \lambda_3)' = E(W)$. It then follows that the moment estimates of the parameters, that is, of $\xi = (\sigma_\gamma^2, \sigma_\epsilon^2, \phi)'$, are obtained by solving the estimating equations

$$W - \lambda = 0, \tag{3.2.18}$$

where, the components λ_u's for $u = 1, 2, 3$ are

$$\begin{aligned} \lambda_1 &= E\left(\frac{1}{S}\sum_{s=1}^{S}(y_s - \mu_s)^2\right) \\ &= \sigma_\gamma^2 + \sigma_\epsilon^2 + \frac{\phi\sigma_\gamma^2}{S}\sum_{s=1}^{S}(n_s - 1), \text{ from } (2.3.9) \\ &= \sigma_\gamma^2 + \sigma_\epsilon^2 + \frac{\phi\sigma_\gamma^2}{S}(N - S), \end{aligned} \tag{3.2.19a}$$

$$\begin{aligned} \lambda_2 &\cong \frac{E\left(\sum_{s=1}^{S-1}(y_s - \mu_s)(y_{s+1} - \mu_{s+1})/(S-1)\right)}{E\left(\sum_{s=1}^{S}(y_s - \mu_s)^2/S\right)} \\ &= \frac{\sigma_\gamma^2}{\lambda_1}\sum_{s=1}^{S-1}\left(\frac{1}{\sqrt{n_s n_{s+1}}}\left[n_{s,s+1} + (n_{s,s+1}(n_{s,s+1} - 1)\right.\right. \\ &\quad \left.\left. + n_{s,s+1}\overline{n}_s + n_{s,s+1}\overline{n}_{s+1} + \widetilde{n}_{s,s+1})\phi\right]\right), \text{ from } (2.3.15) \\ &= \frac{\sigma_\gamma^2}{\lambda_1}\lambda_{21}, \end{aligned} \tag{3.2.19b}$$

$$\begin{aligned}\lambda_3 &\cong \frac{E\left(\sum_{s=1}^{S-2}(y_s-\mu_s)(y_{s+2}-\mu_{s+2})/(S-2)\right)}{E\left(\sum_{s=1}^{S}(y_s-\mu_s)^2/S\right)}\\ &= \frac{\sigma_\gamma^2}{\lambda_1}\sum_{s=1}^{S-2}\left(\frac{1}{\sqrt{n_s n_{s+2}}}[n_{s,s+2}+(n_{s,s+2}(n_{s,s+2}-1)\right.\\ &\quad \left.+n_{s,s+2}\overline{n}_s+n_{s,s+2}\overline{n}_{s+2}+\widetilde{n}_{s,s+2})\phi]\right),\ \text{from}\ \ (2.3.15)\\ &= \frac{\sigma_\gamma^2}{\lambda_1}\lambda_{31}, \end{aligned} \tag{3.2.19c}$$

respectively, where, $N=\sum_{s=1}^{S} n_s$ in (3.2.19a), also in (3.2.19b)

$$\lambda_{21}=\sum_{s=1}^{S-1}\left(\frac{1}{\sqrt{n_s n_{s+1}}}[n_{s,s+1}+(n_{s,s+1}(n_{s,s+1}-1)+n_{s,s+1}\overline{n}_s+n_{s,s+1}\overline{n}_{s+1}+\widetilde{n}_{s,s+1})\phi]\right),$$

and in (3.2.19c)

$$\lambda_{31}=\sum_{s=1}^{S-2}\left(\frac{1}{\sqrt{n_s n_{s+2}}}[n_{s,s+2}+(n_{s,s+2}(n_{s,s+2}-1)+n_{s,s+2}\overline{n}_s+n_{s,s+2}\overline{n}_{s+2}+\widetilde{n}_{s,s+2})\phi]\right).$$

Let $\hat{\xi}_{MM}=(\hat{\sigma}_\gamma^2,\hat{\sigma}_\epsilon^2,\hat{\phi})'$ denote the moment estimator of ξ which is the solution of equation (3.2.18). This solution may be obtained iteratively by using the customary Newton-Raphson iterative equation

$$\hat{\xi}_{MM}(r+1)=\hat{\xi}_{MM}(r)+(P)_{(r)}^{-1}(W-\lambda)_{(r)}, \tag{3.2.20}$$

where $(.)_{(r)}$ denotes the expression within brackets is evaluated at $\hat{\xi}_{MM}(r)$. In (3.2.20), P is the 3×3 derivative matrix of λ with respect to ξ, that is,

$$P = \begin{pmatrix} \frac{\partial\lambda_1}{\partial\sigma_\gamma^2} & \frac{\partial\lambda_1}{\partial\sigma_\epsilon^2} & \frac{\partial\lambda_1}{\partial\phi} \\ \frac{\partial\lambda_2}{\partial\sigma_\gamma^2} & \frac{\partial\lambda_2}{\partial\sigma_\epsilon^2} & \frac{\partial\lambda_2}{\partial\phi} \\ \frac{\partial\lambda_3}{\partial\sigma_\gamma^2} & \frac{\partial\lambda_3}{\partial\sigma_\epsilon^2} & \frac{\partial\lambda_3}{\partial\phi} \end{pmatrix}. \quad (3.2.21)$$

Consequently, by writing the equations (3.2.19a),(3.2.19b) and (3.2.19c) for λ_1,λ_2, and λ_3 respectively, one obtains the formulas for the elements of the derivative matrix P in equation (3.2.21) as

$$\frac{\partial\lambda_1}{\partial\sigma_\gamma^2} = 1 + \frac{\phi}{S}(N-S), \quad \frac{\partial\lambda_1}{\partial\sigma_\epsilon^2} = 1, \quad \frac{\partial\lambda_1}{\partial\phi} = \frac{\sigma_\gamma^2}{S}(N-S),$$

$$\frac{\partial\lambda_2}{\partial\sigma_\gamma^2} = \frac{\sigma_\epsilon^2}{\lambda_1^2}\lambda_{21}, \quad \frac{\partial\lambda_2}{\partial\sigma_\epsilon^2} = -\frac{\sigma_\gamma^2}{\lambda_1^2}\lambda_{21}, \quad \frac{\partial\lambda_2}{\partial\phi} = \frac{\sigma_\gamma^2}{\lambda_1}\lambda_{22} - \frac{\sigma_\gamma^4\lambda_{21}}{S\lambda_1^2}(N-S),$$

with

$$\lambda_{22} = \sum_{s=1}^{S-1} \frac{1}{\sqrt{n_s n_{s+1}}} \left[n_{s,s+1}(n_{s,s+1}-1) + n_{s,s+1}\overline{n}_s + n_{s,s+1}\overline{n}_{s+1} + \widetilde{n}_{s,s+1}\right],$$

and

$$\frac{\partial\lambda_3}{\partial\sigma_\gamma^2} = \frac{\sigma_\epsilon^2}{\lambda_1^2}\lambda_{31}, \quad \frac{\partial\lambda_3}{\partial\sigma_\epsilon^2} = -\frac{\sigma_\gamma^2}{\lambda_1^2}\lambda_{31}, \quad \frac{\partial\lambda_3}{\partial\phi} = \frac{\sigma_\gamma^2}{\lambda_1}\lambda_{32} - \frac{\sigma_\gamma^4\lambda_{31}}{S\lambda_1^2}(N-S),$$

with

$$\lambda_{32} = \sum_{s=1}^{S-2} \frac{1}{\sqrt{n_s n_{s+2}}} \left[n_{s,s+2}(n_{s,s+2} - 1) + n_{s,s+2}\overline{n}_s + n_{s,s+2}\overline{n}_{s+2} + \widetilde{n}_{s,s+2}\right].$$

3.3 Maximum Likelihood Estimation of the Parameters

Recall that the spatial linear mixed model in (3.1.1), in matrix and vector notations, may be written as

$$Y = X\beta + U^*\widetilde{G} + \epsilon. \tag{3.3.1}$$

Note that, it is convenient to deal with the covariance matrix of $U^*\widetilde{G}$ instead of $\widetilde{G}$. Here U^* is a constant coefficient matrix as defined in (3.1.1). Let Σ_γ denote the covariance matrix of $U^*\widetilde{G}$. That is, $U^*\widetilde{G} \sim N(0, \Sigma_\gamma)$ where $\Sigma_\gamma = \sigma_\gamma^2 V : S \times S$ with

$$V = (v_{rs}), \qquad v_{rs} = \begin{cases} 1 + \dfrac{2}{n_s} \displaystyle\sum_{j_s < j'_s}^{n_s} \phi_{j_s j'_s}(s) & \text{if } r = s, \\ \dfrac{1}{\sqrt{n_r n_s}} \displaystyle\sum_{j,} \sum_{k \in f_r \cup f_s} \delta_{jk}\phi^*_{jk} & \text{otherwise,} \end{cases} \tag{3.3.2}$$

where, δ_{rs} and ϕ^*_{rs} are defined in (2.1.1) and (2.1.3b) respectively, and for $j = k$, $\phi^*_{jj} = 1$.

Furthermore in (3.3.1), we write $\epsilon \sim N(0, \Sigma_\epsilon)$, where $\Sigma_\epsilon = \sigma_\epsilon^2 I_S : S \times S$. To simplify the estimation of the model parameters rewrite the mixed model in (3.3.1) as

$$Y = X\beta + \tilde{\epsilon} \text{ or } Y \sim N(X\beta, \Sigma) \tag{3.3.3}$$

where, β is the regression parameter vector, and Σ has the form

$$\begin{aligned} \Sigma &= \Sigma_\gamma + \Sigma_\epsilon \\ &= \sigma_\gamma^2 V + \sigma_\epsilon^2 I_S, \end{aligned} \tag{3.3.4}$$

that is,

$$\Sigma = (\sigma_{rs}) \text{ and } \sigma_{rs} = \begin{cases} \sigma_\gamma^2 \left[1 + \dfrac{2}{n_s} \displaystyle\sum_{j_s < j_s'}^{n_s} \phi_{j_s j_s'}(s) \right] + \sigma_\epsilon^2 & \text{if } r = s, \\ \\ \dfrac{1}{\sqrt{n_r n_s}} \displaystyle\sum \sum_{j,\ k\ \in f_r \cup f_s} \delta_{jk} \phi_{jk}^* \sigma_\gamma^2 & \text{otherwise.} \end{cases} \tag{3.3.5}$$

Now let ψ be a vector of all distinct scale and correlation parameters in the model. Suppose that ψ is of dimension $q \times 1$.

Note that, it is easy to write the likelihood function following (3.3.3). That is,

$$f(\beta, \psi \mid y) = \frac{1}{(2\pi)^{S/2} |\Sigma|^{1/2}} \exp\left\{ -\frac{1}{2} (y - X\beta)' \Sigma^{-1} (y - X\beta) \right\} \tag{3.3.6}$$

where S is the dimension of the response vector. Thus, the log likelihood function for β and ψ is given by

$$\begin{aligned} l(\beta, \psi \mid y) &= -\frac{S}{2}ln(2\pi) - \frac{1}{2}ln|\Sigma| - \frac{1}{2}(y - X\beta)'\Sigma^{-1}(y - X\beta), \\ &= c - \frac{1}{2}ln|\Sigma| - \frac{1}{2}\left\{y'\Sigma^{-1}y - 2y'\Sigma^{-1}X\beta + \beta'X'\Sigma^{-1}X\beta\right\}, \quad (3.3.7) \end{aligned}$$

where c is a constant. By differentiating the log-likelihood with respect to the regression parameter vector β we obtain

$$\frac{\partial l}{\partial \beta} = X'\Sigma^{-1}Y - X'\Sigma^{-1}X\beta, \quad (3.3.8)$$

and the derivatives with respect to scale and correlation parameters ψ_i for $i = 1, \cdots, q$, are given by

$$\begin{aligned} \frac{\partial l}{\partial \psi_i} &= -\frac{1}{2}\frac{\partial ln|\Sigma|}{\partial \psi_i} - \frac{1}{2}(Y - X\beta)'\frac{\partial \Sigma^{-1}}{\partial \psi_i}(Y - X\beta) \\ &= -\frac{1}{2}tr\left[\frac{\partial ln|\Sigma|}{\partial \Sigma} \times \frac{\partial \Sigma}{\partial \psi_i}\right] - \frac{1}{2}(Y - X\beta)'\frac{\partial \Sigma^{-1}}{\partial \psi_i}(Y - X\beta) \\ &= -\frac{1}{2}tr\left[\Sigma^{-1}\Sigma_{(i)}\right] - \frac{1}{2}(Y - X\beta)'\Sigma^{(i)}(Y - X\beta), \quad (3.3.9) \end{aligned}$$

where $\Sigma_{(i)} = \frac{\partial \Sigma}{\partial \psi_i}$, $\Sigma^{(i)} = \frac{\partial \Sigma^{-1}}{\partial \psi_i} = -\Sigma^{-1}\Sigma_{(i)}\Sigma^{-1}$ and ψ_i is the i^{th} component of ψ.

Hence, the MLE for β and ψ_i for $i = 1, \cdots, q$ are obtained by solving

$$\frac{\partial l}{\partial \beta} = X'\Sigma^{-1}Y - X'\Sigma^{-1}X\beta = 0, \quad (3.3.10)$$

and

$$\frac{\partial l}{\partial \psi_i} = -\frac{1}{2} tr\left[\Sigma^{-1}\Sigma_{(i)}\right] - \frac{1}{2}(y - X\beta)'\Sigma^{(i)}(y - X\beta) = 0. \qquad (3.3.11)$$

Note that, for known Σ, the MLE of β has a simple form as

$$\hat{\beta}_{ML} = \left(X'\Sigma^{-1}X\right)^{-1} X'\Sigma^{-1}y \qquad (3.3.12)$$

However, it is clear from (3.3.11) that one does not have a closed form formula for the MLE of ψ_i. That is, it requires solving the non linear equation for ψ_i by using iterative technique, such as Fisher scoring algorithm. For the purpose, we compute the second order derivative for $i, j = 1, \cdots, q$ as

$$l_{\psi_i\psi_j} = \frac{\partial l}{\partial \psi_i \partial \psi_j} = -\frac{1}{2}\left(tr\left[\Sigma^{-1}\Sigma_{(ij)} + \Sigma^{(j)}\Sigma_{(i)}\right] + (y - X\beta)'\Sigma^{(ij)}(y - X\beta)\right) (3.3.13)$$

with $\Sigma_{(ij)} = \dfrac{\partial \Sigma_{(i)}}{\partial \psi_j}$ and,

$$\begin{aligned}
\Sigma^{(ij)} &= \frac{\partial \Sigma^{(i)}}{\partial \psi_j} \\
&= -\frac{\partial}{\partial \psi_j}\left(\Sigma^{-1}\Sigma_{(i)}\Sigma^{-1}\right) \\
&= -\left[\frac{\partial \Sigma^{-1}}{\partial \psi_j}\Sigma_{(i)}\Sigma^{-1} + \Sigma^{-1}\frac{\partial \Sigma_{(i)}}{\partial \psi_j}\Sigma^{-1} + \Sigma^{-1}\Sigma_{(i)}\frac{\partial \Sigma^{-1}}{\partial \psi_j}\right] \\
&= -\left[\Sigma^{(j)}\Sigma_{(i)}\Sigma^{-1} + \Sigma^{-1}\Sigma_{(ij)}\Sigma^{-1} + \Sigma^{-1}\Sigma_{(i)}\Sigma^{j}\right] \\
&= -\left[-\Sigma^{-1}\Sigma_{(j)}\Sigma^{-1}\Sigma_{(i)}\Sigma^{-1} + \Sigma^{-1}\Sigma_{(ij)}\Sigma^{-1} - \Sigma^{-1}\Sigma_{(i)}\Sigma^{-1}\Sigma_{(j)}\Sigma^{-1}\right] \\
&= \Sigma^{-1}\left[\Sigma_{(j)}\Sigma^{-1}\Sigma_{(i)} + \Sigma_{(i)}\Sigma^{-1}\Sigma_{(j)} - \Sigma_{(ij)}\right]\Sigma^{-1}.
\end{aligned}$$

Next we obtain

$$\begin{aligned}
E\left(l_{\psi_i\psi_j}\right) &= -\frac{1}{2}tr\left[\Sigma^{-1}\Sigma_{(ij)} + \Sigma^{(j)}\Sigma_{(i)}\right] - \frac{1}{2}E\left((y-X\beta)'\Sigma^{(ij)}(y-X\beta)\right) \\
&= -\frac{1}{2}tr\left[\Sigma^{-1}\Sigma_{(ij)} + \Sigma^{(j)}\Sigma_{(i)}\right] - \frac{1}{2}E\left(tr\Sigma^{(ij)}(y-X\beta)(y-X\beta)'\right) \\
&= -\frac{1}{2}tr\left[\Sigma^{-1}\Sigma_{(ij)} + \Sigma^{(j)}\Sigma_{(i)}\right] - \frac{1}{2}tr\left[\Sigma^{(ij)}\Sigma\right] \\
&= -\frac{1}{2}tr\left[\Sigma^{-1}\Sigma_{(ij)} + \Sigma^{(j)}\Sigma_{(i)}\right] - \frac{1}{2}tr\left[\Sigma^{-1}\left[\Sigma_{(j)}\Sigma^{-1}\Sigma_{(i)} + \Sigma_{(i)}\Sigma^{-1}\Sigma_{(j)} - \Sigma_{(ij)}\right]\right] \\
&= -\frac{1}{2}tr\left[\Sigma^{-1}\Sigma_{(ij)} - \Sigma^{-1}\Sigma_{(j)}\Sigma^{-1}\Sigma_{(i)}\right. \\
&\qquad \left. + \Sigma^{-1}\Sigma_{(j)}\Sigma^{-1}\Sigma_{(i)} + \Sigma^{-1}\Sigma_{(i)}\Sigma^{-1}\Sigma_{(j)} - \Sigma^{-1}\Sigma_{(ij)}\right] \\
&= -\frac{1}{2}tr\left[\Sigma^{-1}\Sigma_{(i)}\Sigma^{-1}\Sigma_{(j)}\right].
\end{aligned}$$

Thus, we obtain Fisher's score matrix

$$B_\psi = -E\left(l^{(2)}(\beta,\psi \mid y)\right) = -E\left(l_{\psi_i\psi_j}\right) \tag{3.3.14}$$

and the $(i,j)^{\text{th}}$ element of B_ψ is t_{ij} with

$$t_{ij} = \frac{1}{2}tr\left[\Sigma^{-1}\Sigma_{(i)}\Sigma^{-1}\Sigma_{(j)}\right]. \tag{3.3.15}$$

Now for known β, the MLE's $(\hat{\psi}_i)$ of ψ_i for $i = 1, \cdots, q$, can be obtain by solving the maximum likelihood estimating equation (3.3.11). Let $\hat{\psi} = (\hat{\psi}_1, \cdots, \hat{\psi}_q)'$ be the MLE of ψ. This solution may be reached by using the iterative equation method. Given the value of $\hat{\psi}_{ML}(t)$ at the t^{th} iteration, $\hat{\psi}_{ML}(t+1)$ is obtained by solving

$$\hat{\psi}_{ML}(t+1) = \hat{\psi}_{ML}(t) + \left[B_\psi^{-1}\left(\frac{\partial l}{\partial \psi}\right)\right]_{(t)}, \tag{3.3.16}$$

where $[\cdot]_{(t)}$ denotes that the expression within brackets is evaluated at $\hat{\psi}_{ML}(t)$, $\frac{\partial l}{\partial \psi}$ is evaluated from (3.3.9) and B_{ψ}^{-1} is the inverse of B_{ψ} defined in (3.3.14).

Thus, to obtain MLE $\hat{\beta}_{ML}$ of regression parameter vector β and the MLE $\hat{\psi}_{ML}$ of all distinct scale parameters in ψ we may use the following steps:

Step 1: For suitable initial values of ψ_i's ($i = 1, \cdots, q$) estimate β by using (3.3.12).

Step 2: Using β estimate from Step 1, we compute $\hat{\psi}$ by (3.3.16).

Step 3: Estimate of ψ from Step 2 is used in Step 1 to obtain an improved estimate of β which is further used in Step 2 for improved estimate of ψ.

These three Steps constitutes a cycle of iterations and the cycles continue until convergence.

We remark that for the estimation of the variance components in Σ_{γ} matrix, there exists an approach where $\widetilde{G}$ are predicted first by using the so called BLUP (Best Linear Unbiased Predictor) approach and these estimates are used for the estimation of the variance components see for example Searle, Casella, and McCulloch (1992, Section 3.4). This approach has, however convergence problems specially for binary and count data setup. See for example, the discussion by Sutradhar (2011, Chapter 4, p. 66). For this reason, and also because we will deal with binary data in Chapter 4, we do not follow the BLUP based approach.

3.3.1 When Random Effects are Independent

In practice there may be some situations where it is reasonable to assume that the random effects in the spatial region $\mathcal{S}$ are mutually independent. That is, $\phi^*_{jk} = \text{cov}(\gamma^*_j, \gamma^*_k) = 0$. We simplify the likelihood based iterative equation (3.3.16) for this special case.

Note that, for the computation of iterative equation (3.3.16), we need to compute B_ψ and $\frac{\partial l}{\partial \psi}$ for this special case. However it is clear from (3.3.15) and (3.3.9) that B_ψ and $\frac{\partial l}{\partial \psi}$ need the formula for Σ and $\Sigma_{(i)}$. For this purpose we first give the formulas for Σ and $\Sigma_{(i)}$, as follows. Here Σ matrix contains two scale parameters, that is, $q = 2$ and $\psi = (\psi_1, \psi_2)' = (\sigma^2_\gamma, \sigma^2_\epsilon)'$.

3.3.1.1 Computation of Σ matrix

In the present independent case $\phi^*_{jk} = 0$ for $j \neq k$. This also implies that , $\phi^*_{j_s j'_s} = 0$ for $j_s < j'_s$. But $\phi^*_{jj} = 1$ always. Thus by (3.3.2) the elements of V matrix has the formulas

$$V = (v_{rs}), \quad v_{rs} = \begin{cases} 1 & \text{if } r = s, \\ \dfrac{n_{rs}}{\sqrt{n_r n_s}} & \text{otherwise,} \end{cases} \tag{3.3.17}$$

yielding $\Sigma = \sigma^2_\gamma V \; + \; \sigma^2_\epsilon I_S$ from (3.3.5) as

$$\Sigma = (\sigma_{rs}) \text{ and } \sigma_{rs} = \begin{cases} \sigma^2_\gamma + \sigma^2_\epsilon & \text{if } r = s, \\ \dfrac{n_{rs}}{\sqrt{n_r n_s}} \sigma^2_\gamma & \text{otherwise.} \end{cases} \tag{3.3.18}$$

3.3.1.2 Computation of $\Sigma_{(i)}$

From (3.3.18) it is straightforward that for $\psi_1 = \sigma^2_\gamma$ and $\psi_2 = \sigma^2_\epsilon$,

$$\Sigma_{(1)} = \frac{\partial \Sigma}{\partial \psi_1} = (\sigma_{rs(1)}) \text{ with } \sigma_{rs(1)} = \begin{cases} 1 & \text{if } r = s \\ \dfrac{n_{rs}}{\sqrt{n_r n_s}} & \text{otherwise,} \end{cases}$$

and

$$\Sigma_{(2)} = \frac{\partial \Sigma}{\partial \psi_2} = (\sigma_{sk(2)}) \text{ with } \sigma_{rs2)} = \begin{cases} 1 & \text{if } r = s \\ 0 & \text{otherwise.} \end{cases}$$

3.3.2 When Random Effects Follow a Familial Correlation Structure: EQC/Exchangeble Model

As opposed to the independent setup discussed in **3.2.2**, there may be situations where pairwise random effects can be either independent (depending on the distance between two spatial locations) or equi-correlated (within a specified familial distance). To be specified, when k^{th} and l^{th} locations belong to f_s (s^{th} family), it follows from (2.3.4) and (2.3.5) that

$$\phi_{j_s j'_s} \;=\; \text{corr}(\tilde{\gamma}_{sj_s}, \tilde{\gamma}_{sj'_s}) \;=\; \delta_{kl}\phi^*_{kl} \;=\; \phi_{kl}(s) \;=\; \phi$$

always, because they are within a specified familial distance. Further for $r \neq s$ and $k \in f_r$ and $l \in f_s$ we write

$$\phi_{j_r j_s} \;=\; \text{corr}(\tilde{\gamma}_{rj_r}, \tilde{\gamma}_{sj_s}) \;=\; \delta_{kl}\phi^*_{kl},$$

yielding

$$\phi_{j_r j_s} = \begin{cases} \phi^*_{kl} = \phi & \text{if } \; d^*_{kl} \leq d^*, \\ 0 & \text{otherwise.} \end{cases}$$

Next in this equi-correlations setup, $q = 3$ and $\psi = (\psi_1, \psi_2, \psi_3)' = (\sigma^2_\gamma, \sigma^2_\epsilon, \phi)'$. Similar to last the section we now provide the formulas for Σ and $\Sigma_{(i)}$ in terms of ψ_1, ψ_2 and ψ_3.

3.3.2.1 Computation of Σ matrix

When random effects are EQC with correlation parameter ϕ, in a similar way as in (3.3.17) we can obtain the elements of V matrix from (3.3.2) as

$$v_{rs} = \begin{cases} 1 + (n_s - 1)\phi & \text{if } r = s, \\ \dfrac{1}{\sqrt{n_r n_s}} \left\{ n_{rs} \left[1 + (n_{rs} - 1 + \overline{n}_r + \overline{n}_s)\,\phi \right] + \widetilde{n}_{rs}\phi \right\} & \text{otherwise,} \end{cases} \tag{3.3.19}$$

yielding the elements of the covariance matrix Σ in (3.3.5) given by

$$\sigma_{rs} = \begin{cases} \left[1 + (n_s - 1)\phi\right] \sigma_\gamma^2 \; + \; \sigma_\epsilon^2 & \text{if } r = s, \\ \dfrac{1}{\sqrt{n_r n_s}} \left\{ n_{rs} \left[1 + (n_{rs} - 1 + \overline{n}_r + \overline{n}_s)\,\phi \right] + \widetilde{n}_{rs}\phi \right\} \sigma_\gamma^2 & \text{otherwise.} \end{cases} \tag{3.3.20}$$

3.3.2.2 Computation of $\Sigma_{(i)}$

From (3.3.20) it is straightforward that for $i = 1, 2, 3$ we can obtain

$\Sigma_{(1)} = \dfrac{\partial \Sigma}{\partial \psi_1} = (\sigma_{rs(1)})$ with

$$\sigma_{rs(1)} = \begin{cases} 1 + (n_s - 1)\phi & \text{if } r = s, \\ \dfrac{1}{\sqrt{n_r n_s}} \left\{ n_{rs} \left[1 + (n_{rs} - 1 + \overline{n}_r + \overline{n}_s)\,\phi \right] + \widetilde{n}_{rs}\phi \right\} & \text{otherwise.} \end{cases} \tag{3.3.21}$$

Next, we obtain $\Sigma_{(2)} = \dfrac{\partial \Sigma}{\partial \psi_2} = (\sigma_{rs(2)})$ with

$$\sigma_{rs(2)} = \begin{cases} 1 & \text{if } r = s \\ 0 & \text{otherwise,} \end{cases} \tag{3.3.22}$$

and $\Sigma_{(3)} = \dfrac{\partial \Sigma}{\partial \psi_3} = (\sigma_{rs(3)})$ with

$$\sigma_{rs(3)} = \begin{cases} (n_s - 1)\sigma_\gamma^2 & \text{if } r = s, \\ \dfrac{1}{\sqrt{n_r n_s}}\{n_{rs}(n_{rs} - 1 + \overline{n}_r + \overline{n}_s) + \widetilde{n}_{rs}\}\sigma_\gamma^2 & \text{otherwise.} \end{cases} \tag{3.3.23}$$

3.4 A Simulation Study

Recall that s denotes a location of events belonging to a spatial region $\mathcal{S}$. That is $s \in \mathcal{S}$. Also recall from (2.1.7) that, y_s is the associated measurement from the s^{th} spatial location given by

$$\begin{aligned} y_s &= u_s'\alpha + z_s'\theta + \frac{1}{\sqrt{n_s}}\sum_{j_s=1}^{n_s}\widetilde{\gamma}_{sj_s} + \epsilon_s \\ &= x_s'\beta + \frac{1}{\sqrt{n_s}}\sum_{j_s=1}^{n_s}\widetilde{\gamma}_{sj_s} + \epsilon_s \end{aligned} \tag{3.4.1}$$

where, $u_s = (u_{s1}, \cdots, u_{sp_1})'$ is a p_1-dimensional fixed covariate vector containing for example, the epidemiological or demographic information from the s^{th} location, and $z_s = (z_{s1}, \cdots, z_{sp_2})'$ is a p_2-dimensional deterministic (or location dependent) vector of covariate containing the environmental information from the s^{th} location. Here α and θ are the fixed regression effects of u_s and z_s on y_s, respectively, that is $\beta = (\alpha', \theta')'$ is the effect of $x_s' = (u_s', z_s')$ on y_s. Also in (3.4.1), $\widetilde{\gamma}_{sj_s}$ are random effects of n_s locations belonging to the s^{th} family, f_s. Furthermore, as mentioned before ϵ_s are model errors and we assume that $\epsilon_s \overset{iid}{\sim} (0, \sigma_\epsilon^2)$.

3.4.1 Selection of Fixed Covariates

In this simulation study, we choose $S = 500$ locations. With regard to the fixed covariates, we choose $p_1 = 3$ and the associated covariates $u_s = (u_{s1}, u_{s2}, u_{s3})'$ as follows:

1. Intercept covariate:

$$u_{s1} = 1, \quad \text{for} \quad s = 1, 2, \cdots, S$$

2. Fixed epidemiological binary covariate (such as old or new spatial location)

$$u_{s2} = \begin{cases} 1 & \text{if} \quad s \quad \text{is in old category,} \\ 0 & \text{if} \quad s \quad \text{is in new category,} \end{cases}$$

and

3. Another epidemiological covariate (Geographical, say)

$$u_{s3} = \begin{cases} 0 & \text{if} \quad 1 \leq s \leq S/8, \quad \text{(locations are on high ground, for example),} \\ 1 & \text{if} \quad S/8 + 1 \leq s \leq 3S/4, \quad \text{(on plane ground),} \\ 0 & \text{if} \quad 3S/4 + 1 \leq s \leq S, \quad \text{(on high ground).} \end{cases}$$

For environmental type covariate z_s such as to understand the wind effects due to relative positions, we choose two sets of categorical variables each with three categories which may be represented by two categorical variables. To be specific to accommodate for example, the winds from backward (or left) side of a location covering 180^0 we consider the first set of categorical variables represented by two dummy variables (z_{s1}, z_{s2}) defined as:

$$(z_{s1}, z_{s2}) = \begin{cases} (1,0) & \text{if } 135^0 < \omega < 225^0, \\ (0,1) & \text{if } 90^0 < \omega < 135^0, \\ (0,0) & \text{if } 225^0 < \omega < 270^0, \end{cases}$$

where, ω is the angle between s^{th} and its neighboring (backward) locations of events.

Similarly to accommodate for example, the winds from forward (or right) side of a location covering 180^0 we consider the second set of categorical variables represented by two other dummy variables (z_{s3}, z_{s4}) defined as:

$$(z_{s3}, z_{s4}) = \begin{cases} (1,0) & \text{if } 315^0 < \omega < 360^0, \quad \& \quad 0 < \psi < 45^0 \\ (0,1) & \text{if } 45^0 < \omega < 90^0, \\ (0,0) & \text{if } 270^0 < \omega < 315^0, \end{cases}$$

for which, ω is the angle between s^{th} and its neighboring (forward) locations of events. For the fixed regression effects, we chose $\alpha = (\alpha_1, \alpha_2, \alpha_3)'$ and $\theta = (\theta_1, \theta_1, \theta_2, \theta_3, \theta_4)'$, that is,

$$\beta = (\alpha', \theta')' \equiv (0.3,\ 0.5, -0.5,\ 0.6,\ 0.4,\ 0.5,\ 0.2)' \tag{3.4.2}$$

Note that, we have chosen these components of β from some practical point of view. For example, $\alpha_2 = 0.5$ indicates positive effects of older or aged plants on the yields.

3.4.2 Selection of Model Errors

The model error ϵ_s in (3.4.1) is given as

$$\epsilon_s \stackrel{iid}{\sim} N(0, \sigma_\epsilon^2) \tag{3.4.3}$$

As far as the error variance σ_ϵ^2 is concerned, we consider

$$\sigma_\epsilon^2 \equiv (0.5,\ 1.0,\ 2.0). \tag{3.4.4}$$

3.4.3 Selection of Independent Random Effects

Consider γ_s^* as

$$\gamma_s^* \stackrel{iid}{\sim} N(0, \sigma_\gamma^2). \tag{3.4.5}$$

Under this assumption in (3.4.5), it follows that

$$\tilde{\gamma}_{sj_s} = \gamma_{j_s}^* \stackrel{iid}{\sim} N(0, \sigma_\gamma^2) \text{ for } j_s \in f_s. \tag{3.4.6}$$

For values of σ_γ^2, we select

$$\sigma_\gamma^2 \equiv (0.75,\ 1.0,\ 1.5). \tag{3.4.7}$$

Note that, here we have chosen relatively large values for σ_γ^2 because it is important to examine whether the estimation methodology works for such large values, given that it is understands to that no such technical problems arises for small values.

3.4.3.1 Simulated Estimates Under Independent Random Effects Structure

Once the spatial data y_s is generated using (3.4.1) based on regression parameters from (3.4.2), model error variance from (3.4.4) and random error variance from (3.4.7), we now proceed for the estimation of these parameters (β, σ_ϵ^2 and σ_γ^2) following the GLS approach discussed in Section 3.2 and the maximum likelihood method discussed in Section 3.3.

Note that the estimating formulas involve the specific form for the Σ matrix given by (3.2.5). To obtain this specific form under the present spatial linear sequence setup, one needs to know n_{rs} the number of common members to both the families at the r^{th} and the s^{th} locations. For convenience, we provide these values along with the values of n_r as follows:

The number n_r for r^{th} family using figure 3.1 is given by

$$n_r = \begin{cases} 3 & \text{for } r = 1, S, \\ 4 & \text{for } r = 2, S-1, \\ 5 & \text{for } r = 3, \cdots, S-2, \end{cases} \tag{3.4.8}$$

and n_{rs} the number of members common to both families at the r^{th} and s^{th} locations are given as follows:

For $r = 1$ and $s = 2, \cdots, S$

$$n_{1s} = \begin{cases} 3 & \text{for } |1-s| = 1, \\ 3 & \text{for } |1-s| = 2, \\ 2 & \text{for } |1-s| = 3 \\ 1 & \text{for } |1-s| = 4. \\ 0 & \text{otherwise.} \end{cases} \tag{3.4.9}$$

For $r = 2$,$s = 3, \cdots, S$

$$n_{2s} = \begin{cases} 4 & \text{for } |2-s| = 1, \\ 3 & \text{for } |2-s| = 2, \\ 2 & \text{for } |2-s| = 3 \\ 1 & \text{for } |2-s| = 4, \\ 0 & \text{otherwise.} \end{cases} \tag{3.4.10}$$

For $r = 3, \cdots, S-2$, and $s = 4, \cdots, S-1$

$$n_{rs} = \begin{cases} 4 & \text{for } |r-s| = 1, \\ 3 & \text{for } |r-s| = 2, \\ 2 & \text{for } |r-s| = 3 \\ 1 & \text{for } |r-s| = 4, \\ 0 & \text{otherwise}, \end{cases} \tag{3.4.11}$$

and for the remaining pairwise locations, the number of common members are

$$\begin{aligned} n_{S-4,S} &= 1, \\ n_{s-3,S} &= 2, \\ n_{S-2,S} &= 3, \\ n_{S-1,S} &= 3, \\ n_{r,S-1} &= 0, \qquad \text{for } r = 1, 2 \cdots, S-6, \\ n_{rS} &= 0, \qquad \text{for } r = 1, 2 \cdots, S-5. \end{aligned} \tag{3.4.12}$$

For the GLS estimation of β, we use (3.2.2), where the Σ matrix was constructed by using σ_γ^2, σ_ϵ^2, n_r $(r = 1, \cdots, S)$ and n_{rs} $r \neq s$, $(r, s = 1, \cdots, S)$ as explained above, where n_r and n_{rs} are known based on the spatial distance design. The parameters involved in the Σ matrix, that is, σ_γ^2 and σ_ϵ^2 are estimated by the method of moments following the moment equations (3.2.12) and (3.2.13).

Next for maximum likelihood estimation of the parameters, we use the estimating formula (3.3.12) for the regression parameter β which is same as the GLS based estimating formulas for β in (3.2.2). Now because β is estimated for a known Σ matrix and this matrix is a function of σ_γ^2 and σ_ϵ^2 apart from n_r and n_{rs}, we obtain the maximum likelihood estimates of these scale parameters σ_γ^2 and σ_ϵ^2 by solving the likelihood estimating equation (3.3.11). Note that these non-linear equations are solved by using the iterative equation (3.3.16).

The data generation and estimation of the parameters are repeated 1000 times. The simulated means (SMs) and simulated standard errors (SSEs) of the estimators are presented in the following tables from Table 3.1 to Table 3.4 under the GLS approach and in Table 3.5 under the maximum likelihood approach. Note that the results in 3.1 were computed by using lag 1 based moment estimators, which is most practical. However, to see any benefit of using pooled information we have used up to lag 2, lag 3, and lag 4 to find the results in 3.2, 3.3, and 3.4 respectively. But the results do not indicate any significant difference.

Table 3.1: **The SMs and SSEs of the GLS estimates of the regression parameter and moment estimates for the variance components using sample lag 1 correlation with true regression parameter values chosen as $\beta = (\alpha_1, \alpha_2, \alpha_3, \theta_1, \theta_2, \theta_3, \theta_4)' \equiv (0.3, 0.5, -0.5, 0.6, 0.4, 0.5, 0.2)'$ and for selected values of the variance components σ^2_ϵ and σ^2_γ.**

(a) Estimates of the regression parameters

σ^2_ϵ	σ^2_γ	σ^2	Quantity	Regression parameters						
				α_1	α_2	α_3	θ_1	θ_2	θ_3	θ_4
1.0	0.25	1.25	SM	0.287	0.499	-0.499	0.606	0.408	0.506	0.205
			SSE	0.226	0.116	0.135	0.178	0.113	0.171	0.212
	0.75	1.75	SM	0.287	0.500	-0.498	0.607	0.409	0.505	0.202
			SSE	0.257	0.120	0.195	0.188	0.117	0.181	0.229
	1.0	2.0	SM	0.287	0.500	-0.498	0.608	0.409	0.505	0.201
			SSE	0.270	0.122	0.219	0.191	0.118	0.185	0.234
	1.5	2.5	SM	0.287	0.500	-0.498	0.608	0.409	0.505	0.200
			SSE	0.295	0.125	0.259	0.196	0.120	0.190	0.242

(b) Estimates of the variance components

σ^2_ϵ	σ^2_γ	σ^2	Quantity	Variance parameters		
				σ^2_ϵ	σ^2_γ	σ^2
1.0	0.25	1.25	SM	0.983	0.241	1.224
			SSE	0.087	0.084	0.081
	0.75	1.75	SM	0.985	0.727	1.712
			SSE	0.096	0.150	0.131
	1.0	2.0	SM	0.986	0.971	1.956
			SSE	0.100	0.183	0.157
	1.5	2.5	SM	0.988	1.457	2.445
			SSE	0.110	0.250	0.213

Table 3.2: **The SMs and SSEs of the GLS estimates of the regression parameter and moment estimates for the variance components using up to sample lag 2 correlation with true regression parameter values chosen as** $\beta = (\alpha_1, \alpha_2, \alpha_3, \theta_1, \theta_2, \theta_3, \theta_4)' \equiv (0.3, 0.5, -0.5, 0.6, 0.4, 0.5, 0.2)'$ **and for selected values of the variance components** σ^2_ϵ **and** σ^2_γ**.**

(a) Estimates of the regression parameters

			Quantity	Regression parameters						
σ^2_ϵ	σ^2_γ	σ^2		α_1	α_2	α_3	θ_1	θ_2	θ_3	θ_4
1.0	0.25	1.25	SM	0.287	0.499	-0.499	0.606	0.408	0.506	0.205
			SSE	0.226	0.116	0.135	0.178	0.113	0.172	0.212
	0.75	1.75	SM	0.287	0.500	-0.498	0.607	0.409	0.505	0.202
			SSE	0.257	0.120	0.195	0.188	0.117	0.181	0.229
	1.0	2.0	SM	0.287	0.500	-0.498	0.608	0.409	0.505	0.201
			SSE	0.270	0.122	0.218	0.192	0.118	0.185	0.233
	1.5	2.5	SM	0.287	0.500	-0.498	0.608	0.409	0.504	0.201
			SSE	0.295	0.125	0.259	0.196	0.120	0.190	0.242

(b) Estimates of the variance components

			Quantity	Variance parameters		
σ^2_ϵ	σ^2_γ	σ^2		σ^2_ϵ	σ^2_γ	σ^2
1.0	0.25	1.25	SM	0.987	0.238	1.224
			SSE	0.083	0.080	0.081
	0.75	1.75	SM	0.985	0.727	1.712
			SSE	0.096	0.150	0.131
	1.0	2.0	SM	0.991	0.964	1.956
			SSE	0.104	0.189	0.157
	1.5	2.5	SM	0.995	1.450	2.445
			SSE	0.120	0.261	0.213

Table 3.3: **The SMs and SSEs of the GLS estimates of the regression parameter and moment estimates for the variance components using uo to sample lag 3 correlation with true regression parameter values chosen as $\beta = (\alpha_1, \alpha_2, \alpha_3, \theta_1, \theta_2, \theta_3, \theta_4)' \equiv (0.3, 0.5, -0.5, 0.6, 0.4, 0.5, 0.2)'$ and for selected values of the variance components σ_ϵ^2 and σ_γ^2.**

(a) Estimates of the regression parameters

			Quantity	Regression parameters						
σ_ϵ^2	σ_γ^2	σ^2		α_1	α_2	α_3	θ_1	θ_2	θ_3	θ_4
1.0	0.25	1.25	SM	0.287	0.499	-0.499	0.606	0.408	0.506	0.205
			SSE	0.226	0.116	0.135	0.178	0.113	0.171	0.213
	0.75	1.75	SM	0.287	0.500	-0.498	0.607	0.409	0.505	0.202
			SSE	0.257	0.120	0.195	0.188	0.117	0.181	0.229
	1.0	2.0	SM	0.287	0.500	-0.498	0.608	0.409	0.505	0.201
			SSE	0.270	0.122	0.218	0.191	0.118	0.185	0.234
	1.5	2.5	SM	0.287	0.500	-0.498	0.608	0.409	0.505	0.200
			SSE	0.295	0.125	0.259	0.196	0.120	0.190	0.242

(b) Estimates of the variance components

			Quantity	Variance parameters		
σ_ϵ^2	σ_γ^2	σ^2		σ_ϵ^2	σ_γ^2	σ^2
1.0	0.25	1.25	SM	0.988	0.236	1.224
			SSE	0.085	0.082	0.081
	0.75	1.75	SM	0.994	0.717	1.712
			SSE	0.106	0.160	0.131
	1.0	2.0	SM	0.997	0.959	1.956
			SSE	0.117	0.199	0.157
	1.5	2.5	SM	0.988	1.457	2.445
			SSE	0.110	0.250	0.213

Table 3.4: **The SMs and SSEs of the GLS estimates of the regression parameter and moment estimates for the variance components using up to sample lag 4 correlation with true regression parameter values chosen as $\beta = (\alpha_1, \alpha_2, \alpha_3, \theta_1, \theta_2, \theta_3, \theta_4)' \equiv (0.3, 0.5, -0.5, 0.6, 0.4, 0.5, 0.2)'$ and for selected values of the variance components σ_ϵ^2 and σ_γ^2.**

(a) Estimates of the regression parameters

			Quantity	Regression parameters						
σ_ϵ^2	σ_γ^2	σ^2		α_1	α_2	α_3	θ_1	θ_2	θ_3	θ_4
1.0	0.25	1.25	SM	0.287	0.499	-0.499	0.606	0.408	0.506	0.205
			SSE	0.226	0.116	0.135	0.178	0.113	0.171	0.212
	0.75	1.75	SM	0.287	0.500	-0.498	0.607	0.409	0.505	0.202
			SSE	0.257	0.120	0.195	0.188	0.117	0.181	0.229
	1.0	2.0	SM	0.287	0.500	-0.498	0.608	0.409	0.505	0.201
			SSE	0.270	0.122	0.218	0.192	0.118	0.185	0.234
	1.5	2.5	SM	0.287	0.500	-0.498	0.608	0.409	0.505	0.200
			SSE	0.295	0.125	0.259	0.196	0.120	0.190	0.242

(b) Estimates of the variance components

			Quantity	Variance parameters		
σ_ϵ^2	σ_γ^2	σ^2		σ_ϵ^2	σ_γ^2	σ^2
1.0	0.25	1.25	SM	0.983	0.241	1.224
			SSE	0.087	0.084	0.081
	0.75	1.75	SM	0.998	0.714	1.712
			SSE	0.124	0.175	0.131
	1.0	2.0	SM	1.003	0.953	1.956
			SSE	0.142	0.219	0.157
	1.5	2.5	SM	1.012	1.432	2.445
			SSE	0.181	0.305	0.213

Table 3.5: **The SMs and SSEs of the ML estimates of the regression and variance components with true regression parameter values chosen as** $\beta = (\alpha_1, \alpha_2, \alpha_3, \theta_1, \theta_2, \theta_3, \theta_4)' \equiv (0.3, 0.5, -0.5, 0.6, 0.4, 0.5, 0.2)'$ **and for selected values of the variance components** σ_ϵ^2 **and** σ_γ^2**.**

(a) ML Estimates of the regression parameters

		Quantity	Regression rarameters						
σ_ϵ^2	σ_γ^2		α_1	α_2	α_3	θ_1	θ_2	θ_3	θ_4
1.0	0.25	SM	0.290	0.500	-0.498	0.602	0.407	0.501	0.196
		SSE	0.229	0.119	0.132	0.177	0.112	0.175	0.204
	0.75	SM	0.287	0.500	-0.498	0.607	0.409	0.505	0.202
		SSE	0.257	0.120	0.195	0.188	0.117	0.181	0.229
	1.0	SM	0.286	0.500	-0.496	0.602	0.408	0.502	0.195
		SSE	0.271	0.124	0.214	0.190	0.116	0.188	0.226
	1.5	SM	0.283	0.500	-0.495	0.601	0.407	0.503	0.195
		SSE	0.295	0.127	0.253	0.195	0.119	0.233	0.242

(b) ML Estimates of the variance components

		Quantity	Variance parameters	
σ_ϵ^2	σ_γ^2		σ_ϵ^2	σ_γ^2
1.0	0.25	SM	0.983	0.242
		SSE	0.082	0.079
	0.75	SM	0.998	0.714
		SSE	0.124	0.175
	1.0	SM	0.981	0.979
		SSE	0.095	0.173
	1.5	SM	0.980	1.471
		SSE	0.101	0.232

The results from Table 3.1 to Table 3.4 show that the model parameters are estimated very well by using the GLS approach. All estimates for regression parameter and variance components appear to be unbiased, except that the variance components estimates become slightly biased when σ_γ^2 is large. However this bias appears to be insignificant. As far as the simulated standard errors of the estimates are concerned, the SSEs of the GLS estimates of the regression estimators appear to increase in a slow rate when σ_γ^2 increases. However, the SSEs of the estimates of the σ_γ^2 in particular get larger when true value of σ_γ^2 gets larger which is expected.

When the result of Table 3.5 obtained under MLE are compared to any of the tables from 3.1 to 3.4 the regression estimates appear to be almost the same. However the maximum likelihood approach produces the estimates of σ_γ^2 with less bias and smaller simulated standard errors as compared to the moment approach. This indicates the optimal behavior of the ML approach in the present spatial regression set up.

3.4.4 Selection of Random Effects: Exchangeable (EQC) Familial Correlation

Recall that in general

$$\gamma_s^* \sim (0, \sigma_\gamma^2) \tag{3.4.13a}$$

and

$$\text{corr}(\gamma_r^*, \gamma_s^*) = \delta_{rs}\phi_{rs}^*. \tag{3.4.13b}$$

Now to develop a equi-correlation structure for the random effects of the member locations of the s^{th} family, that is, to develop

$$\phi_{j_s j_s'}(s) = \text{corr}(\widetilde{\gamma}_{sj_s}, \widetilde{\gamma}_{sj_s'}) = \begin{cases} 1 & \text{for } j_s = j_s' \\ \phi & \text{for } j_s \neq j_s', \end{cases} \tag{3.4.14}$$

one has to develop an appropriate correlation structure among all $\gamma_1^*, \cdots, \gamma_s^*, \cdots, \gamma_S^*$ which will provide the correlations as in (3.4.14) for the members of the s^{th} family.

3.4.4.1 Special Case with Linear Spatial Sequences

To illustrate this development, for simplicity suppose that all s locations are in a linear sequence and they form a family of correlated random effects at a given location (say r) where the distance between the r^{th} and any other locations (say s), that is, $d_{rs}^* \leq d^*$.

This produces a correlation structure for $\gamma_s^*(s = 1, \cdots, S)$ of the form

$$\text{corr}(\gamma_r^*, \gamma_s^*) = \begin{cases} 1 & \text{for } d_{rs}^* = 0 \\ \phi & \text{for } d_{rs}^* \leq d^* \\ 0 & \text{for } d_{rs}^* > d^*, \end{cases} \tag{3.4.15}$$

which generates a band correlation matrix with pairwise correlation ϕ within the band, where the band width is determined by the spatial distance (lag) d^*. We present this situation in the form of following figures.

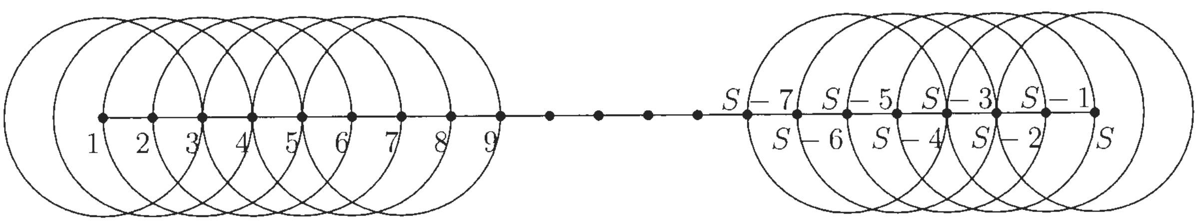

Figure 3.1: Equi-correlation based linear spatial sequences

3.4.4.2 Generation of γ_s^* satisfying (3.4.15)

In this special case, we consider $d^* = 4$ and for $S = 500$ generate $\gamma_1^*, \cdots, \gamma_s^* \cdots, \gamma_S^*$, following the correlation structure (3.4.15). To be specific for $d^* = 4$

$$\text{corr}(\gamma_r^*, \gamma_s^*) = \phi \text{ when } r \neq s \text{ and } d_{rs}^* \leq 4. \tag{3.4.16}$$

For this (3.4.16) to happen, we generate γ_s^* in a sequence as follows:

$$\begin{aligned}
\gamma_1^* &\sim N\left(0, \sigma_\gamma^2\right) \\
\gamma_2^* \mid \gamma_1^* &\sim N\left(\phi\gamma_1^*, \sigma_\gamma^2(1-\phi^2)\right) \\
\vdots \quad &\vdots \quad \vdots \\
\gamma_r^* \mid \gamma_1^*, \cdots, \gamma_{r-1}^* &\sim N\left[\Lambda_{21}^{(r)}\left(\Lambda_{11}^{(r)}\right)^{-1}\gamma_{(r-1)}^*,\ \Lambda_{22}^{(r)} - \Lambda_{21}^{(r)}\left(\Lambda_{11}^{(r)}\right)^{-1}\Lambda_{12}^{(r)}\right]
\end{aligned}$$

where for $r = 2\cdots, 5$,

$$\gamma_{(r-1)}^* = (\gamma_1^*, \cdots, \gamma_{r-1}^*)', \quad \Lambda_{21}^{(r)} = \phi\sigma_\gamma^2 1_{r-1}', \quad \Lambda_{22}^{(r)} = \sigma_\gamma^2, \quad \Lambda_{12}^{(r)} = \left(\Lambda_{21}^{(r)}\right)'$$

and

$$\Lambda_{11}^{(r)} = 1_{r-1}1_{r-1}'\phi\sigma_\gamma^2 + \sigma_\gamma^2(1-\phi)I_{r-1},$$

and for $r = 6, \cdots, S$ the $(r-1)\times(r-1)$ dimension matrix $\Lambda_{11}^{(r)}$ is given by

$$\Lambda_{11}^{(r)} = \left(\lambda_{uv}^{(r)}\right) = \begin{cases} \sigma_\gamma^2 & \text{when } \ u = v \\ \phi\sigma_\gamma^2 & \text{when } \ |u-v| = 1, \cdots, d^* \\ 0 & \text{for } \ |u-v| > d^*, \end{cases}$$

and

$$\Lambda_{21}^{(r)} = \phi\sigma_\gamma^2\left[0 \times 1_{r-1-d^*}', 1_{d^*}'\right], \quad \Lambda_{22}^{(r)} = \sigma_\gamma^2, \quad \Lambda_{12}^{(r)} = \left(\Lambda_{21}^{(r)}\right)'.$$

Now to use (3.4.1) to generate y_s, we need to identify $\widetilde{\gamma}_s = (\widetilde{\gamma}_{s1}, \cdots, \widetilde{\gamma}_{sj_s}, \cdots, \widetilde{\gamma}_{sn_s})'$ under f_s. This identification should be chosen from the following table.

Table 3.6: **Familial random effects corresponding to spatial random effects under the linear sequence with $d^* = 4$**

Family	Family Random Effects	Corresponds to original random effects
f_1	$[\widetilde{\gamma}_{11}, \widetilde{\gamma}_{12}, \widetilde{\gamma}_{13}]$	$[\gamma_1^*(=\widetilde{\gamma}_{11}), \gamma_2^*, \gamma_3^*]$
f_2	$[\widetilde{\gamma}_{21}, \widetilde{\gamma}_{22}, \widetilde{\gamma}_{23}, \widetilde{\gamma}_{24}]$	$[\gamma_2^*(=\widetilde{\gamma}_{21}), \gamma_1^*, \gamma_3^*, \gamma_4^*]$
f_3	$[\widetilde{\gamma}_{31}, \widetilde{\gamma}_{32}, \widetilde{\gamma}_{33}, \widetilde{\gamma}_{34}, \widetilde{\gamma}_{35}]$	$[\gamma_3^*(=\widetilde{\gamma}_{31}), \gamma_1^*, \gamma_2^*, \gamma_4^*, \gamma_5^*]$
$\vdots$	$\vdots$	$\vdots$
$\vdots$	$\vdots$	$\vdots$
f_{498}	$[\widetilde{\gamma}_{498,1}, \widetilde{\gamma}_{498,2}, \widetilde{\gamma}_{498,3}, \widetilde{\gamma}_{498,4}, \widetilde{\gamma}_{498,5}]$	$[\gamma_{498}^*(=\widetilde{\gamma}_{498,1}), \gamma_{496}^*, \gamma_{497}^*, \gamma_{499}^*, \gamma_{500}^*]$
f_{499}	$[\widetilde{\gamma}_{499,1}, \widetilde{\gamma}_{499,2}, \widetilde{\gamma}_{499,3}, \widetilde{\gamma}_{499,4}]$	$[\gamma_{499}^*(=\widetilde{\gamma}_{499,1}), \gamma_{500}^*, \gamma_{497}^*, \gamma_{498}^*]$
f_{500}	$[\widetilde{\gamma}_{500,1}, \widetilde{\gamma}_{500,2}, \widetilde{\gamma}_{500,3}]$	$[\gamma_{500}^*(=\widetilde{\gamma}_{500,1}), \gamma_{499}^*, \gamma_{498}^*]$

3.4.4.3 A Simulation Study Based on Random Effects with Familial (EQC) Correlation Structure

Recall that when the random effects follow a familial correlation structure, the pairwise correlations between two responses are given by (2.3.16), where ϕ is the pairwise correlation between random effects arising from neighboring locations. Note that unlike when the random effects were independent (3.2.5), the variances and covariances of the responses now contain ϕ in addition to n_r, n_{rs}, $\bar{n}_r$, $\bar{n}_s$ and $\widetilde{n}_{rs}$. For convenience we reproduce (see (2.3.16) the formula for variances and covariances here as

$$\sigma_{rs} = \begin{cases} [1 + (n_s - 1)\phi]\,\sigma_\gamma^2 \;+\; \sigma_\epsilon^2 & \text{if } \; r = s, \\ \dfrac{1}{\sqrt{n_r n_s}}\left\{n_{rs}\left[1 + (n_{rs} - 1 + \overline{n}_r + \overline{n}_s)\,\phi\right] + \widetilde{n}_{rs}\phi\right\}\sigma_\gamma^2 & \text{otherwise.} \end{cases} \tag{3.4.17}$$

Further note that the values for n_r and n_{rs} remain the same as in the previous simulation study discussed in Section 3.4.3. The values of the remaining sizes that is, $\bar{n}_r$, $\bar{n}_s$ and $\widetilde{n}_{rs}$ may be computed following the general formula discussed in Section 2.2.2.2. We compute these values for the $d^* = 4$ case as follows.

For $r = 1$ and $s = 2, \cdots, S$

$$\widetilde{n}_{1s} = \begin{cases} 2 & \text{for} \quad |s-1| = 3, \\ 5 & \text{for} \quad |s-1| = 4, \\ 9 & \text{for} \quad |s-1| = 5, \\ 6 & \text{for} \quad |s-1| = 6, \\ 3 & \text{for} \quad |s-1| = 7, \\ 1 & \text{for} \quad |s-1| = 8, \\ 0 & \text{otherwise.} \end{cases} \tag{3.4.18}$$

For $r = 2$ and $s = 3, \cdots, S$

$$\widetilde{n}_{2s} = \begin{cases} 1 & \text{for} \quad |s-2| = 2, \\ 3 & \text{for} \quad |s-2| = 3, \\ 6 & \text{for} \quad |s-2| = 4, \\ 10 & \text{for} \quad |s-2| = 5, \\ 6 & \text{for} \quad |s-2| = 6, \\ 3 & \text{for} \quad |s-2| = 7, \\ 1 & \text{for} \quad |s-2| = 8, \\ 0 & \text{otherwise.} \end{cases} \tag{3.4.19}$$

For $r = 3, \cdots, S-3$, and $s = 4, \cdots, S-2$

$$\widetilde{n}_{rs} = \begin{cases} 1 & \text{for } |s-r| = 2, \\ 3 & \text{for } |s-r| = 3, \\ 6 & \text{for } |s-r| = 4, \\ 10 & \text{for } |s-r| = 5, \\ 6 & \text{for } |s-r| = 6, \\ 3 & \text{for } |s-r| = 7, \\ 1 & \text{for } |s-r| = 8, \\ 0 & \text{otherwise.} \end{cases} \tag{3.4.20}$$

For $r = 1, \cdots, S-2$, and $s = S-1$

$$\widetilde{n}_{r,S-1} = \begin{cases} 1 & \text{for } |S-1-r| = 2, \\ 3 & \text{for } |S-1-r| = 3, \\ 6 & \text{for } |S-1-r| = 4, \\ 10 & \text{for } |S-1-r| = 5, \\ 6 & \text{for } |S-1-r| = 6, \\ 3 & \text{for } |S-1-r| = 7, \\ 1 & \text{for } |S-1-r| = 8, \\ 0 & \text{otherwise.} \end{cases} \tag{3.4.21}$$

and for $r = 1, \cdots, S-1$, and $s = S$

$$\widetilde{n}_{rS} = \begin{cases} 2 & \text{for } |S-r| = 3, \\ 5 & \text{for } |S-r| = 4, \\ 9 & \text{for } |S-r| = 5, \\ 6 & \text{for } |S-r| = 6, \\ 3 & \text{for } |S-r| = 7, \\ 1 & \text{for } |S-r| = 8, \\ 0 & \text{otherwise.} \end{cases} \tag{3.4.22}$$

Next the number of members only from the r^{th} family may be easily computed by using the formula $\bar{n}_r = n_r - n_{rs}$, where the number of n_r and n_{rs} were given in Section **3.4.3.1**. However, for the sake of completeness, we provide the values for $\bar{n}_r$ as follows.

For $r = 1$ and $s = 2, \cdots, S$

$$\bar{n}_1 = \begin{cases} 0 & \text{for } |s-1| \leq 2, \\ |s-1| - 2 & \text{for } 2 < |s-1| \leq 4, \\ 3 & \text{otherwise.} \end{cases} \tag{3.4.23}$$

For $r = 2$ and $s = 3, \cdots, S$

$$\bar{n}_2 = \begin{cases} 0 & \text{for } |s-2| \leq 1, \\ |s-2|-1 & \text{for } 1 < |s-2| \leq 4, \\ 4 & \text{otherwise.} \end{cases} \tag{3.4.24}$$

For $r = 3, \cdots, S-3$, and $s = 4, \cdots, S-2$

$$\bar{n}_r = \begin{cases} |s-r| & \text{for } 1leq|s-r| \leq 4, \\ 5 & \text{otherwise.} \end{cases} \tag{3.4.25}$$

For $r = 3, \cdots, S-2$, and $s = S-1$

$$\bar{n}_r = \begin{cases} |S-1-r| & \text{for } |S-1-r| \leq 4, \\ 5 & \text{otherwise,} \end{cases} \tag{3.4.26}$$

and for $r = 3, \cdots, S-1$, and $s = S$

$$\bar{n}_r = \begin{cases} |S-r| & \text{for } 1 \leq |S-r| \leq 4, \\ 5 & \text{otherwise.} \end{cases} \tag{3.4.27}$$

Also, the number of members only from the s^{th} family is computed as follows:

For $r = 1, 2, \cdots, S-3$, and $s = 2, \cdots, S-2$

$$\bar{n}_s = \begin{cases} |s-r| & \text{for } 1 < |s-r| \leq 4, \\ 5 & \text{otherwise.} \end{cases} \tag{3.4.28}$$

For $r = 1, \cdots, S-2$, and $s = S-1$

$$\bar{n}_{S-1} = \begin{cases} 0 & \text{for } |S-1-r| \leq 1, \\ |S-1-r|-1 & \text{for } 1 < |S-1-r| \leq 4, \\ 4 & \text{otherwise,} \end{cases} \quad (3.4.29)$$

and for $r = 1, \cdots, S-1$, and $s = S$

$$\bar{n}_{S} = \begin{cases} 0 & \text{for } |S-r| \leq 2, \\ |S-r|-2 & \text{for } 2 < |S-r| \leq 4, \\ 3 & \text{otherwise.} \end{cases} \quad (3.4.30)$$

Data Generation:

We consider the same covariate design, that is, $x_s = (u_s', z_s')'$ and choose the same true values for β as in Section **3.4.1**. However, as our objective is to examine the effect of familial correlation ϕ for random effects, we choose a moderately large value for $\phi = 0.3$ (given that a moving average order 1 correlation cannot exceed 0.5), and examine the estimation performance for variance parameter $\sigma_\gamma^2 = 0.75$ and 1, and $\sigma_\epsilon^2 = 1.0$.

Note that it is now important to generate the random effects γ_s^* $(s = 1, \cdots, S)$ such that they follow a moving familial or band structure with correlations either ϕ or 0.

For this, for the selected value of $\phi = 0.3$, we generate the random effects following Section **3.4.4.2**. Alternatively, one may generate the S-dimensional random effects using, for example, the FORTRAN 90 IMSL subroutine RNMVN, where Cholesky decomposition is used for standardization. Once the random effects are generated, we use them in the model (3.4.1) to generate the correlated responses $\{y_s\}$. For the spatial size we choose $S = 500$.

Estimation Performance

When the number of parameters increases, it becomes relatively difficult to write appropriate moment equations for all parameters. However, the ML approach does not have this problem in the present setup. We, thus, consider the ML approach and examine its performance in estimating all parameters β, σ_γ^2, σ_ϵ^2 and ϕ. To be specific we use the estimating formula (3.3.12) for the regression parameter β which is same as the GLS based estimating formulas for β in (3.2.2). Because β is estimated for a known Σ matrix and this matrix is a function of σ_γ^2 , σ_ϵ^2 and ϕ apart from n_r, n_s, n_{rs}, $\bar{n}_r$, $\bar{n}_s$ and $\widetilde{n}_{rs}$, in a given simulation, we use suitable initial values such as $\sigma_\gamma^2 = 0.1$, $\sigma_\epsilon^2 = 0.1$ and $\phi = 0.0$, to obtain the β estimate at the first step, We then use the estimate of β to obtain the maximum likelihood estimates of these scale correlation parameters σ_γ^2, σ_ϵ^2 and ϕ by solving the likelihood estimating equations (3.3.11). Note that these non-linear equations are solved by using the iterative equation (3.3.16). These estimates are then used in (3.3.12) to obtain improved estimate of β. This constitutes a cycle which continues until convergence. This we repeat for 50 simulations. Note that, because we have to conduct a large spatial sequence with $S = 500$, each simulation takes a considerable computing time requiring a relative large amount of computing time for 50 simulations. However, given time is not a problem, we would obtain better estimates if simulation number is increased.

The simulated estimates along with the standard errors are presented in Table 3.7. The results from the Table 3.7 indicate that the ML approach performs well in estimating all parameters including ϕ parameter. For example for this $\phi = 0.3$ case when $\sigma_\epsilon^2 = 1.0$ and $\sigma_\gamma^2 = 0.75$, the estimates for the components of β were found to be $\hat{\beta} = (0.271, 0.500, -0.559, 0.590, 0.399, 0.509, 0.201)'$ which are close to the true values of the regression parameters. The ϕ parameter value, (that is, $\phi = 0.3$) was estimated as 0.28 which is quite satisfactory. The σ_γ^2 parameter was found to be slightly under estimated as 0.69, whereas σ_ϵ^2 was estimated much better as 0.98.

Note that we have also carried out a simulation study based on 500 simulations with results shown in Table 3.8, whereas the above simulation results were based on 50 simulations. When the results in Table 3.8 are compared to Table 3.7, as expected, these appears to be a big improvement in estimates, they are being much closer to the true values. For example, for $\sigma_\epsilon^2 = 1.0$, $\sigma_\gamma^2 = 1.0$, and $\phi = 0.3$ the estimates from Table 3.7 are found to be 0.974, 0.971 and 0.296 respectively, whereas these estimates from Table 3.8 are 0.988, 1.005 and 0.309 respectively, showing a big bias reduction. This happened, however with same or slight larger variances.

Table 3.7: **The SMs and SSEs of the ML estimates of the regression and scale parameters with true regression parameter values chosen as $\beta = (\alpha_1, \alpha_2, \alpha_3, \theta_1, \theta_2, \theta_3, \theta_4)' \equiv (0.3, 0.5, -0.5, 0.6, 0.4, 0.5, 0.2)'$ and for selected values of the variance components σ_γ^2 and σ_ϵ^2 when $\phi = 0.3$.**

(a) ML estimates of the regression parameters

		Quantity	Regression parameters						
σ_ϵ^2	σ_γ^2		α_1	α_2	α_3	θ_1	θ_2	θ_3	θ_4
1.0	0.75	SM	0.275	0.500	-0.559	0.590	0.399	0.509	0.201
		SSE	0.322	0.120	0.312	0.224	0.127	0.146	0.245
	1.0	SM	0.275	0.498	-0.573	0.588	0.399	0.509	0.202
		SSE	0.341	0.124	0.344	0.231	0.131	0.148	0.254

(b) ML estimates of the variance and correlation parameters

		Quantity	Variance and correlation		
σ_ϵ^2	σ_γ^2		σ_ϵ^2	σ_γ^2	ϕ
1.0	0.75	SM	0.981	0.687	0.281
		SSE	0.109	0.373	0.182
	1.0	SM	0.974	0.971	0.296
		SSE	0.096	0.212	0.107

Table 3.8: **The SMs and SSEs of the ML estimates of the regression and scale parameters with true regression parameter values chosen as** $\beta = (\alpha_1, \alpha_2, \alpha_3, \theta_1, \theta_2, \theta_3, \theta_4)' \equiv (0.3, 0.5, -0.5, 0.6, 0.4, 0.5, 0.2)'$ **and for selected values of the variance components** σ^2_γ **and** σ^2_ϵ **when** $\phi = 0.3$**.**

(a) ML estimates of the regression parameters

		Quantity	Regression parameters						
σ^2_ϵ	σ^2_γ		α_1	α_2	α_3	θ_1	θ_2	θ_3	θ_4
1.0	0.75	SM	0.286	0.495	-0.495	0.600	0.403	0.507	0.209
		SSE	0.330	0.109	0.328	0.197	0.112	0.185	0.257
	1.0	SM	0.286	0.494	-0.495	0.602	0.404	0.506	0.209
		SSE	0.362	0.111	0.373	0.200	0.111	0.188	0.260

(b) ML estimates of the variance and correlation parameters

		Quantity	Variance and correlation		
σ^2_ϵ	σ^2_γ		σ^2_ϵ	σ^2_γ	ϕ
1.0	0.75	SM	0.982	0.768	0.310
		SSE	0.034	0.213	0.146
	1.0	SM	0.988	1.005	0.309
		SSE	0.097	0.245	0.126

We have also estimated the regression and variance parameters by ignoring ϕ, that is, by using $\phi = 0$ (same as assuming random effects are independent). The results based on 500 simulations are presented in Table 3.9. It is clear from the table that the approach produces highly biased estimates specially for the variance components σ_ϵ^2 and σ_γ^2. This is however, not surprising because of the fact that $\phi = 0$ does not mean that the responses are pairiwse independent. Also, $\phi = 0$ produces incorrect variances for the responses. Consequently, the MLE for σ_ϵ^2 and σ_γ^2 are bound to be adversely affected. This would also happen if one uses Weighted Generalized Leaset Squares (WGLS) technique, when $\phi = 0$ would lead to wrong weights.

Table 3.9: **The SMs and SSEs of the ML estimates of the regression and scale parameters with true regression parameter values chosen as $\beta = (\alpha_1, \alpha_2, \alpha_3, \theta_1, \theta_2, \theta_3, \theta_4)' \equiv (0.3, 0.5, -0.5, 0.6, 0.4, 0.5, 0.2)'$ and for selected value of the variance components $\sigma_\gamma^2 = 1.0$ and $\sigma_\epsilon^2 = 1.0$ when $\phi = 0.3$.**

(a) ML estimates of the regression parameters

		Quantity	Regression parameters						
σ_ϵ^2	σ_γ^2		α_1	α_2	α_3	θ_1	θ_2	θ_3	θ_4
1.0	1.0	SM	0.294	0.494	-0.507	0.597	0.402	0.506	0.199
		SSE	0.366	0.124	0.369	0.203	0.121	0.193	0.246

(b) ML estimates of the variance and correlation parameters

		Quantity	Variance and correlation	
σ_ϵ^2	σ_γ^2		σ_ϵ^2	σ_γ^2
1.0	1.0	SM	0.841	1.930
		SSE	0.057	0.256

The results based on 500 simulations are presented in Table 3.10 by considering random effects are independent, providing satisfactory results.

Table 3.10: **The SMs and SSEs of the ML estimates of the regression and scale parameters with true regression parameter values chosen as $\beta = (\alpha_1, \alpha_2, \alpha_3, \theta_1, \theta_2, \theta_3, \theta_4)' \equiv (0.3, 0.5, -0.5, 0.6, 0.4, 0.5, 0.2)'$ and for selected value of the variance components $\sigma^2_\gamma = 1.0$ and $\sigma^2_\epsilon = 1.0$ when $\phi = 0.0$**

(a) ML estimates of the regression parameters

		Quantity	Regression parameters						
σ^2_ϵ	σ^2_γ		α_1	α_2	α_3	θ_1	θ_2	θ_3	θ_4
1.0	1.0	SM	0.289	0.501	-0.499	0.603	0.408	0.498	0.190
		SSE	0.281	0.124	0.222	0.189	0.119	0.190	0.228

(b) ML estimates of the variance and correlation parameters

		Quantity	Variance and correlation		
σ^2_ϵ	σ^2_γ		σ^2_ϵ	σ^2_γ	ϕ
1.0	1.0	SM	0.982	0.975	0.012
		SSE	0.103	0.260	0.060

Chapter 4

Spatial Mixed Models for Binary Response

There are situations in practice when binary responses are collected from neighboring and hence correlated locations. For example, in a forestry study one may be interested to examine the effects of certain suitable covariates on the damage status (yes or no) of a tree, perhaps done by insects in a harsh weather, in a selected region of study. In fact some authors such as Rathbun and Cressie (1994) have developed a survival point process for a long leaf pine forest in Southern Georgia, USA, where survival (yes or no) rates were studied over a period of nine years from 1979 to 1987. To be specific, we refer to Rathbun and Cressie (1994 Section 5.2) for a spatial temporal binary model. For a given year, this model reduces to the spatial binary model. For this case by suppressing the time τ notation, Rathbun and Cressie's (1994 equation (16)) spatial binary probability model in our notation of previous chapters, may be written as

$$Pr\left(M_{rj_r} = 1 \mid x_r, x_s, \|\mathbf{s}_{rj_r} - \mathbf{s}_{sj_s}\| < d^*\right) = \frac{\exp\left[x_r'\beta + \widetilde{W}_{rs}\right]}{1 + \exp\left[x_r'\beta + \widetilde{W}_{rs}\right]} \tag{4.0.1}$$

where $\widetilde{W}_{rs} = \eta_{rs}(x_s, \|\mathbf{s}_{rj_r} - \mathbf{s}_{sj_s}\| < d^*, r \neq s,\ r, s = 1, \cdots, S;\ j_r = 1, \cdots, n_r;\ j_s = 1, \cdots, n_s)$, M_{rj_r} is the binary response of the j_r^{th} member of the r^{th} family, $\widetilde{W}_{rs}$ is a known function say, η_{rs} of covariates (x_s) from other locations belonging to f_s, these locations in f_s being correlated with the locations belonging to f_r depending on the distance criterion $(< d^*)$. Note that unlike these authors, we have denoted the responses by y_r $(r = 1. \cdots, S)$ and in our notation f_r is the r^{th} family consisting of n_r members. Thus $y_r \equiv M_{r1}$, M_{r1} being the binary response for the first member of the r^{th} family. However instead of $\widetilde{W}_{rs}$ we will use a linear function of random effects from the f_r family to influence y_r (on top of x_r) and write

$$P(Y_r = 1 \mid f_r, f_s) = \frac{\exp\left[x_r'\beta + \frac{1}{\sqrt{n_r}} 1_{n_r}' \widetilde{\gamma}_{r(s)}\right]}{1 + \exp\left[x_r'\beta + \frac{1}{\sqrt{n_r}} 1_{n_r}' \widetilde{\gamma}_{r(s)}\right]},\ r \neq s \tag{4.0.2}$$

where some of the components of $\widetilde{\gamma}_{r(s)}' = (\widetilde{\gamma}_{r1(s)}, \cdots, \widetilde{\gamma}_{rn_r(s)})$ for example, suppressing the subscript (s), $\widetilde{\gamma}_{rj_r}$ may be correlated with some components of $\widetilde{\gamma}_{s(r)}' = (\widetilde{\gamma}_{s1(r)}, \cdots, \widetilde{\gamma}_{sn_s(r)})$, say $\widetilde{\gamma}_{rj_r}$ depending on the distance between the j_r^{th} member of the r^{th} family ($j_r \in f_r$) and j_s^{th} being the member of the s^{th} family ($j_s \in f_s$) of locations whether $d_{j_r j_s} \leq d^*$ or $d_{j_r j_s} > d^*$. Note that using $\widetilde{\gamma}_{r(s)}$ in the formula for $P(Y_r = 1)$ is justified because we are interested to compute all possible pairwise correlations, s being another location and the common random effects between r^{th} and s^{th} locations will cause the correlation between y_r and y_s. Following (4.0.2) we may write the model for the binary response y_s from the s^{th} location where a family f_s formed at this s^{th} location. To be specific

$$P(Y_s = 1 \mid f_s, f_r) = \frac{\exp\left[x_s'\beta + \frac{1}{\sqrt{n_s}} 1_{n_s}' \widetilde{\gamma}_{s(r)}\right]}{1 + \exp\left[x_s'\beta + \frac{1}{\sqrt{n_s}} 1_{n_s}' \widetilde{\gamma}_{s(r)}\right]}, \quad r \neq s \tag{4.0.3}$$

Let $W_{r(s)}^* = \frac{1}{\sqrt{n_r}} 1_{n_r}' \widetilde{\gamma}_{r(s)}$ and $W_{s(r)}^* = \frac{1}{\sqrt{n_s}} 1_{n_s}' \widetilde{\gamma}_{s(r)}$. With regard to the distribution of the random effects we use the same assumption as for spatial linear mixed model (2.1.7). Thus by (2.1.8) - (2.1.10) we write

$$E(W_{r(s)}^*) = 0, \tag{4.0.4}$$

and

$$\begin{aligned} \text{var}\left(W_{r(s)}^*\right) &= \text{var}\left(\frac{1}{\sqrt{n_r}} 1_{n_r}' \widetilde{\gamma}_{r(s)}\right) \\ &= \sigma_\gamma^2 \left[1 + \frac{2}{n_r} \sum_{j_r < j_r'}^{n_r} \phi_{j_r j_r'}\right]. \end{aligned} \tag{4.0.5}$$

In the special case when pairwise random effects are equi-correlated, that is, $\phi_{j_r j'_r} = \phi$, for $j_r \neq j'_r$, this variance reduces to

$$\text{var}(W^*_{r(s)}) = \sigma^2_\gamma[1 + (n_r - 1)\phi] = \sigma^*_{rr}(n_r, \sigma^2_\gamma, \phi), \text{ (say)} \tag{4.0.6}$$

Furthermore, the linear functions of the random effects defined for the r^{th} and s^{th} locations, namely $W^*_{r(s)}$ and $W^*_{s(r)}$ are correlated and for the special equi-correlated random effects, their covariance, by (2.3.16), has the form

$$\begin{aligned} \text{cov}\left(W^*_{r(s)}, W^*_{s(r)}\right) &= \frac{1}{\sqrt{n_r n_s}} \{n_{rs}[1 + (n_{rs} - 1 + \overline{n}_r + \overline{n}_s)\phi] + \widetilde{n}_{rs}\phi\}\sigma^2_\gamma \\ &= \sigma^*_{rs}(n_r, n_s, n_{rs}, \bar{n}_r, \bar{n}_s, \widetilde{n}_{rs}, \sigma^2_\gamma, \phi), \text{ (say).} \end{aligned} \tag{4.0.7}$$

4.1 Basic Properties

For convenience we consider the standardized spatial linear function

$$W_{r(s)} = \frac{W^*_{r(s)}}{\sigma^{*\frac{1}{2}}_{rr}}, \tag{4.1.1}$$

where $\sigma^*_{rr} = \text{var}(W^*_{r(s)}) = \sigma^2_\gamma[1 + (n_r - 1)\phi]$ as in (4.0.6), and rewrite the probability function (4.0.2) as

$$P(Y_r = 1 \mid f_r, f_s) = \frac{\exp\left[x'_r\beta + \sigma^{*\frac{1}{2}}_{rr} W_{r(s)}\right]}{1 + \exp\left[x'_r\beta + \sigma^{*\frac{1}{2}}_{rr} W_{r(s)}\right]} \tag{4.1.2}$$

where $W_{r(s)} \sim N(0, 1)$.

Before proceeding towards the development of estimation techniques for the parameters β, σ_γ^2 and ϕ involved in the binary mixed model (4.0.2),(4.0.3) and (4.1.2) we provide the basic properties such as the conditional means variances and covariances in Section 4.1.1 and corresponding unconditional first and second order moments in Section 4.1.2. Note that these marginal and product moments of order two are helpful in understanding the mean and correlation structures of the response under the model, and along with the product moments of order three and four, they may be exploited to develop the desired GQL estimation approach for regression and scale parameters. The later product moments of order three and four are discussed in Section 4.2.5 in the context of estimating the scale parameters σ_γ^2 and ϕ.

4.1.1 Conditional First and Second Order Moments

In notation used in (4.1.2), we write the conditional moments as in the following lemma.

Lemma 4.1.1 Conditional on $W_{r(s)}$, that is, conditional on the random effects involved in f_r, the mean and the variance of the response y_r are given by

$$E\left(Y_r \mid W_{r(s)}\right) = \frac{\exp\left[x_r'\beta + \sigma_{rr}^{*\frac{1}{2}} W_{r(s)}\right]}{1+\exp\left[x_r'\beta + \sigma_{rr}^{*\frac{1}{2}} W_{r(s)}\right]} = \pi_r^*(W_{r(s)}), \quad \text{(say)} \tag{4.1.3}$$

and

$$\text{var}\left(Y_r \mid W_{r(s)}\right) = \pi_r^*(W_{r(s)})\left[1 - \pi_r^*(W_{r(s)})\right]. \qquad (4.1.4)$$

Next condition on both $W_{r(s)}$ and $W_{s(r)}$, that is, conditional on the random effects involved in f_r and f_s, the covariance between y_r and y_s for $r \neq s$ is given by

$$\begin{aligned}
\text{cov}\left[(Y_r, Y_s) \mid W_{r(s)}, W_{s(r)}\right] &= E\left(Y_r Y_s \mid W_{r(s)}, W_{s(r)}\right) - \pi_r^* \pi_s^* \\
&= E\left(Y_r \mid W_{r(s)}\right) E\left(Y_s \mid W_{s(r)}\right) - \pi_r^* \pi_s^* \\
&= \pi_r^* \pi_s^* - \pi_r^* \pi_s^* \\
&= 0. \qquad (4.1.5)
\end{aligned}$$

4.1.2 Unconditional First and Second Order Moments

The corresponding unconditional mean, variance and covariance are given in the following lemma:

Lemma 4.1.2 By (4.1.3) the unconditional mean and variance of the spatial binary response y_r are given by

$$
\begin{aligned}
E(Y_r) &= E_{W_{r(s)}} E(Y_r \mid W_{r(s)}) \\
&= E_{W_{r(s)}} \pi_r^*(W_{r(s)}) \\
&= \int \pi_r^*(W_{r(s)}) \Phi(W_{r(s)}) dW_{r(s)} \\
&= \pi_r \equiv \mu_r, \qquad (4.1.6)
\end{aligned}
$$

and

$$
\begin{aligned}
\text{var}(Y_r) &= E\left(Y_r^2\right) - [E(Y_r)]^2 \\
&= E\left(Y_r^2\right) - \pi_r^2.
\end{aligned}
$$

Because Y_r is binary, $E\left(Y_r^2\right) = E\left(Y_r\right)$. Thus

$$
\begin{aligned}
\text{var}(Y_r) &= E\left(Y_r\right) - \pi_r^2 \\
&= \pi_r - \pi_r^2 \\
&= \pi_r(1 - \pi_r) \qquad (4.1.7)
\end{aligned}
$$

where, $\Phi(.)$ in (4.1.6) is the standardized normal density. Note that this integral in (4.1.6) is difficult to evaluate. However, there exists a simulation approach (Jiang (1998), Sutradhar (2011) p. 123) as well as a binomial approximation approach to solve this integration. Because the generation of the standard normal variable, namely

$W_{r(s)} \sim N(0,1)$, is simple, we follow the simulation approach to compute the expectation in (4.1.6).

Let $W_{r(s)}(j)$ denote the j^{th} $(j = 1, \cdots, J)$ simulated value for $W_{r(s)}$, where J is large enough such as $J = 500$ or more. We may then approximate the mean in (4.1.6) as

$$\begin{aligned} E(Y_r) &\cong \frac{1}{J}\sum_{j=1}^{J} \pi_r^* \left(W_{r(s)}(j)\right) \\ &= \frac{1}{J}\sum_{j=1}^{J} \frac{\exp\left[x_r'\beta + \sigma_{rr}^{*\frac{1}{2}} W_{r(s)}(j)\right]}{1+\exp\left[x_r'\beta + \sigma_{rr}^{*\frac{1}{2}} W_{r(s)}(j)\right]} \\ &= \widetilde{\pi}_r. \end{aligned} \quad (4.1.8)$$

and hence the approximate variance in (4.1.7) reduces to

$$\text{var}(Y_r) = \widetilde{\pi}_r(1-\widetilde{\pi}_r) = \widetilde{\sigma}_{rr}, \quad (4.1.9)$$

Lemma 4.1.3 The unconditional covariance between two spatial responses y_r and y_s from locations r and s $(r \neq s)$ is given by

$$\begin{aligned} \sigma_{rs} = \text{cov}(Y_r, Y_s) &= E(Y_r Y_s) - \pi_r \pi_s \\ &= \lambda_{rs} - \pi_r \pi_s, \end{aligned} \quad (4.1.10)$$

where

$$\begin{aligned}
\lambda_{rs} &= E(Y_r Y_s) \\
&= \int \frac{\exp\left[x_r'\beta + \sigma_{rr}^{*\frac{1}{2}} W_{r(s)}\right]}{1+\exp\left[x_s'\beta + \sigma_{rr}^{*\frac{1}{2}} W_{r(s)}\right]} \frac{\exp\left[x_s'\beta + \sigma_{ss}^{*\frac{1}{2}} W_{s(r)}\right]}{1+\exp\left[x_s'\beta + \sigma_{ss}^{*\frac{1}{2}} W_{s(r)}\right]} \\
&\quad \widetilde{\Phi}(W_{r(s)}, W_{s(r)}) dW_{r(s)} dW_{s(r)}, \qquad (4.1.11)
\end{aligned}$$

$\widetilde{\Phi}(W_{r(s)}, W_{s(r)})$ being the bivariate normal density for $W_{r(s)}$ and $W_{s(r)}$, where

$$E(W_{r(s)}) = E(W_{s(r)}) = 0,$$

$$\text{var}(W_{r(s)}) = \text{var}(W_{s(r)}) = 1$$

and correlation between $W_{r(s)}$ and $W_{s(r)}$ is given by

$$\begin{aligned}
\rho_{rs}^* &= \text{corr}\left(W_{r(s)}, W_{s(r)}\right) \\
&= \text{corr}\left(\frac{W_{r(s)}^*}{\sigma_{rr}^{*\frac{1}{2}}}, \frac{W_{s(r)}^*}{\sigma_{ss}^{*\frac{1}{2}}}\right) \\
&= \frac{1}{\sigma_{rr}^{*\frac{1}{2}} \sigma_{ss}^{*\frac{1}{2}}} \text{cov}\left(W_{r(s)}^*, W_{s(r)}^*\right),
\end{aligned}$$

by (4.1.1). It then follows by (4.0.6) and (4.0.7) that

$$\rho_{rs}^* = \frac{\sigma_{rs}^*}{\left[\sigma_{rr}^* \sigma_{ss}^*\right]^{\frac{1}{2}}}, \qquad (4.1.12)$$

which is same as the corr $\left(W_{r(s)}^*, W_{s(r)}^*\right)$. Note that similar to (4.1.8) λ_{rs} in (4.1.11) can be approximated as

$$\widetilde{\lambda}_{rs} = \frac{1}{J} \sum_{j=1}^{J} \pi_r^* \left(W_{r(s)}(j)\right) \pi_s^* \left(W_{s(r)}(j)\right), \qquad (4.1.13)$$

where

$$\begin{pmatrix} W_{r(s)} \\ W_{s(r)} \end{pmatrix} \sim N_2 \left[\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho^*_{rs} \\ \rho^*_{rs} & 1 \end{pmatrix} \right] \tag{4.1.14}$$

yielding

$$\text{cov}(Y_r, Y_s) \;\cong\; \widetilde{\lambda}_{rs} - \widetilde{\pi}_r \widetilde{\pi}_s \;=\; \widetilde{\sigma}_{rs} \tag{4.1.15}$$

4.1.2.1 Generation of two Correlated Standardized Normal Values

Let

$$\Sigma_{(rs)} = \begin{pmatrix} 1 & \rho^*_{rs} \\ \rho^*_{rs} & 1 \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{4.1.16}$$

we now find

$$\Sigma^{\frac{1}{2}}_{(rs)} = \begin{pmatrix} l_{11} & l_{12} \\ l_{21} & l_{22} \end{pmatrix}, \tag{4.1.17}$$

such that $\Sigma^{\frac{1}{2}}_{(rs)} \Sigma^{\frac{1}{2}}_{(rs)} = \Sigma_{(rs)}$. Let $\tau = a + d = 2$, $g^2 = \delta = ad - bc = (1 - \rho^{*2}_{rs}) > 0$ and $t^2 = \tau + 2g = 2 + 2\sqrt{1 - \rho^2_{rs}}$. It then follows (Somayya (1997)) that

$$\begin{aligned} l_{11} \;=\; \frac{a+g}{t} \;&=\; \frac{1 + \sqrt{1 - \rho^{*2}_{rs}}}{\left[2\{1 + \sqrt{1 - \rho^{*2}_{rs}}\}\right]} \\ &=\; \sqrt{\frac{1 + \sqrt{1 - \rho^{*2}_{rs}}}{2}}, \end{aligned} \tag{4.1.18}$$

$$l_{12} = \frac{b}{t} = \frac{\rho^*_{rs}}{\left[2\{1+\sqrt{1-\rho^{*2}_{rs}}\}\right]} = l_{21}, \tag{4.1.19}$$

and

$$\begin{aligned} l_{22} = \frac{d+g}{t} &= \frac{1+\sqrt{1-\rho^{*2}_{rs}}}{\left[2\{1+\sqrt{1-\rho^{*2}_{rs}}\}\right]} \\ &= \sqrt{\frac{1+\sqrt{1-\rho^{*2}_{rs}}}{2}} = l_{11}. \end{aligned} \tag{4.1.20}$$

Consequently

$$\Sigma^{-\frac{1}{2}}_{W_{(rs)}} \begin{pmatrix} W_{r(s)} \\ W_{s(r)} \end{pmatrix} = \begin{pmatrix} \widetilde{W}_{r(s)} \\ \widetilde{W}_{s(r)} \end{pmatrix} \sim N_2 \left[\begin{pmatrix} 0 \\ 0 \end{pmatrix}, I_2 \right], \tag{4.1.21}$$

implying that

$$\begin{aligned} \begin{pmatrix} W_{r(s)} \\ W_{s(r)} \end{pmatrix} &= \Sigma^{\frac{1}{2}}_{rs} \begin{pmatrix} \widetilde{W}_{r(s)} \\ \widetilde{W}_{s(r)} \end{pmatrix} \\ &= \begin{pmatrix} l_{11} & l_{12} \\ l_{12} & l_{11} \end{pmatrix} \begin{pmatrix} \widetilde{W}_{r(s)} \\ \widetilde{W}_{s(r)} \end{pmatrix} \\ &= \begin{bmatrix} l_{11}\widetilde{W}_{r(s)} + l_{12}\widetilde{W}_{s(r)} \\ l_{12}\widetilde{W}_{r(s)} + l_{11}\widetilde{W}_{s(r)} \end{bmatrix}. \end{aligned} \tag{4.1.22}$$

where l_{11}, l_{12} and l_{22} have the formulas as in (4.1.18), (4.1.19) and (4.1.20), respectively.

4.1.2.2 Computational Formula for $\widetilde{\lambda}_{rs}$

Turning back to (4.1.13) and by using (4.1.22) we compute $\widetilde{\lambda}_{rs}$ as

$$\widetilde{\lambda}_{rs} = \frac{1}{J}\sum_{j=1}^{J} \frac{\exp\left[x_r'\beta + \sigma_{rr}^{*\frac{1}{2}}\left\{l_{11}\widetilde{W}_{r(s)}(j) + l_{12}\widetilde{W}_{s(r)}(j)\right\}\right]}{1+\exp\left[x_r'\beta + \sigma_{rr}^{*\frac{1}{2}}\left\{l_{11}\widetilde{W}_{r(s)}(j) + l_{12}\widetilde{W}_{s(r)}(j)\right\}\right]} \frac{\exp\left[x_s'\beta + \sigma_{ss}^{*\frac{1}{2}}\left\{l_{12}\widetilde{W}_{r(s)}(j) + l_{11}\widetilde{W}_{s(r)}(j)\right\}\right]}{1+\exp\left[x_s'\beta + \sigma_{ss}^{*\frac{1}{2}}\left\{l_{12}\widetilde{W}_{r(s)}(j) + l_{11}\widetilde{W}_{s(r)}(j)\right\}\right]} \quad (4.1.23)$$

where $\widetilde{W}_{r(s)}(j) \sim N(0,1)$ and $\widetilde{W}_{s(r)}(j) \sim N(0.1)$, and also $\widetilde{W}_{r(s)}(j)$ and $\widetilde{W}_{s(r)}(j)$ are independent.

Remark that when the parameters β, σ_γ^2 and ϕ are known or estimated, σ_{rr}^*, σ_{ss}^*, l_{11}, and l_{12} become known. Then the computations for $\widetilde{\pi}_r$ by (4.1.8) and $\widetilde{\lambda}_{rs}$ by (4.1.23) are computed by generating two sets of independent normal values, namely $\widetilde{W}_{r(s)}(j)$ and $\widetilde{W}_{s(r)}(j)$ for $j = 1, \cdots, J$.

4.2 Estimation for Correlated Random Effect Based Parametric Spatial Mixed Model

Recall that the present spatial binary response model (4.1.2) involves the regression parameter vector β, the individual random effects σ_γ^2, and the pairwise correlation parameter ϕ. All these parameters are present in the means, variances and covariances of the binary response model. To be specific, we have computed the unconditional mean, that is, $E(Y_r) \cong \widetilde{\pi}_r$ by (4.1.8) for all $r = 1, \cdots, S$ and the unconditional covariance namely $\text{cov}(Y_r, Y_s) \cong \widetilde{\lambda}_{rs} - \widetilde{\pi}_r\widetilde{\pi}_s = \widetilde{\sigma}_{rs}$ by (4.1.15), where these formulas contain β, σ_γ^2 and ϕ. Note that for independent familial binary models, the associated parameters were consistently and efficiently estimated by using the generalized quasi-likelihood (GQL) approach, see for example, Sutradhar (2011, Section 5.2.3). In the present setup, the neighboring families are correlated and far distant familes would be uncorrelated (independent). However, because the correlation structures among the members of the same family as well as between the members of the neighboring families are constructed in the last section, we exploit them here and following Sutradhar (2011), develop the GQL approach for the estimation of β, σ_γ^2 and ϕ. More specifically in the following three subsections, we demonstrate how to develop the marginal GQL estimating equations for the parameters. These marginal equations, for example, the marginal estimating equation for β will be solved by assuming that other parameters σ_γ^2 and ϕ are known. Similarly the marginal estimating equation for σ_γ^2 will be solved by assuming that β and ϕ are known, and so on.

4.2.1 Marginal GQL Estimation for β

Because the regression parameter vector β is of our main interest and because $\widetilde{\sigma}_{rr}$ is a known function of $\widetilde{\pi}_r$, it is sufficient to exploit the first order responses $\{y_r, \quad r = 1, \cdots, S\}$ to estimate β involved in $\{\widetilde{\pi}_r \equiv E(Y_r), \quad r = 1, \cdots, S\}$. Consider

$$y = (y_1, y_2, \cdots, y_S)', \tag{4.2.1}$$

with

$$E(Y) = \widetilde{\pi} = (\widetilde{\pi}_1, \cdots, \widetilde{\pi}_r, \cdots, \widetilde{\pi}_S)'. \tag{4.2.2}$$

Next because

$$\widetilde{\Sigma} = \text{var}(Y) = (\widetilde{\sigma}_{rs}), \tag{4.2.3}$$

where $\widetilde{\sigma}_{rs}$ is constructed in (4.1.15), following Sutradhar (2011, Section 5.2.3) and for known σ^2_γ and ϕ, we solve the GQL estimating equation for β given by

$$\frac{\partial \widetilde{\pi}'}{\partial \beta} \widetilde{\Sigma}^{-1}(y - \widetilde{\pi}) = 0. \tag{4.2.4}$$

Remark that as mentioned above, Sutradhar (2011, Section 5.2.3, equ. (5.52)) has constructed the GQL estimating equation for independent families where binary responses from the members of a given family were correlated. In the present spatial setup, unlike Sutradhar (2011 Section 5.2.3) the binary responses from the neighboring families are likely to be correlated. Thus, in general, families are not treated as independent to each other. However the far distant families would be independent. Because when the location r is far away from the location s, that is, $s >> r$, the far distant families namely f_r and f_s will have $n_{rs} = \widetilde{n}_{rs} = 0$. Consequently, in many practical situations, the $\widetilde{\Sigma} = \text{var}(Y)$ will have a band pattern. That is, for $s >> r$, $\widetilde{\sigma}_{rs}$ becomes zero, making a large number of off diagonal with zeros. This makes the inverse of the $\widetilde{\Sigma}$ matrix ($\widetilde{\Sigma}^{-1}$) manageable, even though $\widetilde{\Sigma}$ is a large dimensional $(S \times S)$ matrix.

Let $\hat{\beta}_{GQL}$ be the solution to the marginal GQL estimating equation (4.2.4). This solution may be obtained where $[\cdot]_{(t)}$ denotes that the expression within the square brackets is evaluated at $\beta = \hat{\beta}_{GQL}(t)$, the estimate obtained for the t^{th} iteration. In (??) the derivative matrix $\frac{\partial \widetilde{\pi}'}{\partial \beta}$ can be computed by using the formula for $\frac{\partial \widetilde{\pi}_r}{\partial \beta}$ from (4.1.8) for all $r = 1, \cdots, S$, that is,

$$\frac{\partial \widetilde{\pi}_r}{\partial \beta} = \frac{1}{J} \sum_{j=1}^{J} \pi_r^*(W_{r(s)}(j))[1 - \pi_r^*(W_{r(s)}(j))]x_r. \qquad (4.2.5)$$

Note that the GQL estimator for β satisfying (4.2.4) is consistent because $E(Y) = \widetilde{\pi}$ which makes the estimating equation (4.2.4) unbiased. Furthermore, because $\widetilde{\Sigma}$ is the true covariance matrix of Y, the β estimator will also be more efficient than any other estimators that uses $\widetilde{\Sigma} = I$ or a working version of $\widetilde{\Sigma}$.

4.2.2 Marginal GQL Estimation for σ_γ^2

For the estimation of σ_γ^2, we exploit all lag zero (squared) and lag one (pairwise product) second order responses. Let

$$u_1 = (y_1^2, \cdots, y_r^2, \cdots, y_S^2)' \tag{4.2.6}$$

and

$$u_2 = (y_1 y_2, \cdots, y_r y_{r+1}, \cdots, y_{S-1} y_S)', \tag{4.2.7}$$

where $y_{r\pm1}$ are the responses from the adjacent neighbors of the r^{th} location. Because $y_r^2 = y_r$, we write $u_1 = y = (y_1, \cdots, y_S)'$. Further let

$$u = (u_1', u_2')', \tag{4.2.8}$$

with

$$E(U) = \widetilde{\lambda} = (\widetilde{\lambda}_1', \widetilde{\lambda}_2')', \tag{4.2.9}$$

where $\widetilde{\lambda}_1 = E(U_1) = (\widetilde{\pi}_1, \cdots, \widetilde{\pi}_S)'$ and $\widetilde{\lambda}_2 = E(U_2) = (\widetilde{\lambda}_{12}, \cdots, \widetilde{\lambda}_{S-1,S})'$. Suppose that we can compute or approximate the covariance matrix for U. Let $\Omega = \text{cov}(U)$ denote this matrix. Then for known β and ϕ we write the second order based GQL estimating equation for σ_γ^2 as

$$\frac{\partial \widetilde{\lambda}'}{\partial \sigma_\gamma^2} \Omega^{-1}(u - \widetilde{\lambda}) = 0, \tag{4.2.10}$$

where $\widetilde{\pi}_r$ in $\widetilde{\lambda}_1$ has the formula given in (4.1.8), and $\widetilde{\lambda}_{rs}$ in $\widetilde{\lambda}_2$ has the formula given in (4.1.23). Note that both $\widetilde{\pi}_r$ $(r = 1, \cdots, S)$ and $\widetilde{\lambda}_{rs}$ $(r \neq s, r, s = 1, \cdots, S)$ are functions of β, σ^2_γ and ϕ. However the estimating equation (4.2.10) requires the derivatives of $\widetilde{\pi}_r$ and $\widetilde{\lambda}_{rs}$ with respect to σ^2_γ only. These derivatives are given in Section 4.2.4. Note that Ω in (4.2.10) is constructed in Section 4.2.5.

Let $\hat{\sigma^2}_{\gamma GQL}$ be the solution to the marginal GQL estimating equation (4.2.10). This solution may be obtained by using the customary Newton Raphson method. Given that value of $\hat{\sigma^2}_{\gamma GQL}(t)$ at the t^{th} iteration, $\hat{\sigma^2}_{\gamma GQL}(t+1)$ is obtained as equation

$$\hat{\sigma^2}_{\gamma GQL}(t+1) = \hat{\sigma^2}_{\gamma GQL}(t) + \left[\frac{\partial \widetilde{\lambda}'}{\partial \sigma^2_\gamma}\Omega^{-1}\frac{\partial \widetilde{\lambda}}{\partial \sigma^2_\gamma}\right]^{-1}_{(t)} \left[\frac{\partial \widetilde{\lambda}'}{\partial \sigma^2_\gamma}\Omega^{-1}(u - \widetilde{\lambda})\right]_{(t)} \tag{4.2.11}$$

where $[\cdot]_{(t)}$ denotes that the expression within brackets is evaluated at $\hat{\sigma^2}_{\gamma GQL}(t)$.

4.2.3 Marginal GQL Estimation for ϕ

For the estimation of ϕ we use the same base statistic u given in (4.2.8) and its mean as in (4.2.9). Then for known β and σ^2_γ we write the GQL estimating equation for ϕ as

$$\frac{\partial \widetilde{\lambda}'}{\partial \phi}\Omega^{-1}(u - \widetilde{\lambda}) = 0, \tag{4.2.12}$$

which is similar to (4.2.10) for σ_γ^2, but these equations are different because the derivatives with respect to ϕ and σ_γ^2 are different.

Let $\hat{\phi}_{GQL}$ be the solution to the marginal GQL estimating equation (4.2.12). This solution may be obtained by using the customary Newton Raphson method. Given that value of $\hat{\phi}_{GQL}(t)$ at the t^{th} iteration, $\hat{\phi}_{GQL}(t+1)$ is obtained as equation

$$\hat{\phi}_{GQL}(t+1) = \hat{\phi}_{GQL}(t) + \left[\frac{\partial\widetilde{\lambda}'}{\partial\phi}\Omega^{-1}\frac{\partial\widetilde{\lambda}}{\partial\phi}\right]^{-1}_{(t)} \left[\frac{\partial\widetilde{\lambda}'}{\partial\phi}\Omega^{-1}(u - \widetilde{\lambda})\right]_{(t)} \tag{4.2.13}$$

where $[\cdot]_{(t)}$, denotes that the expression within brackets is evaluated at $\hat{\phi}_{GQL}(t)$.

4.2.4 Computation of Derivatives

4.2.4.1 Computation of $\frac{\partial\widetilde{\lambda}'}{\partial\sigma_\gamma^2}$

The derivative vector $\frac{\partial\widetilde{\lambda}'}{\partial\sigma_\gamma^2}$ involved in the GQL estimating equation (4.2.10) can be computed by using the derivatives $\frac{\partial\widetilde{\lambda}'_1}{\partial\sigma_\gamma^2}$ and $\frac{\partial\widetilde{\lambda}'_2}{\partial\sigma_\gamma^2}$. However the derivative $\frac{\partial\widetilde{\lambda}'_1}{\partial\sigma_\gamma^2}$ can be computed by obtaining the derivatives using $\frac{\partial\widetilde{\pi}_r}{\partial\sigma_\gamma^2}$ $(r = 1, \cdots, S)$ only, where $\widetilde{\pi}_r$ is given by (4.1.8). Similarly the derivative $\frac{\partial\widetilde{\lambda}'_2}{\partial\sigma_\gamma^2}$ can be computed by using the formula for $\frac{\partial\widetilde{\lambda}_{rs}}{\partial\sigma_\gamma^2}$ from (4.1.23) for all $r \neq s, r, s = 1, \cdots, S$.

Computation of $\frac{\partial \widetilde{\pi}_r}{\partial \sigma_\gamma^2}$:

Notice that in (4.1.8), σ_γ^2 is involved only in σ_{rr}^*, by (4.0.6) which has the formula $\sigma_{rr}^* = \sigma_\gamma^2[1 + (n_r - 1)\phi]$. It then follows that

$$\frac{\partial \widetilde{\pi}_r}{\partial \sigma_\gamma^2} = \frac{1}{J}\sum_{j=1}^{J} \pi_r^*(W_{r(s)}(j))[1 - \pi_r^*(W_{r(s)}(j))]\,[1 + (n_r - 1)\phi]\,\frac{W_{r(s)}(j)}{2\sigma_{rr}^{*\frac{1}{2}}}. \quad (4.2.14)$$

Computation of $\frac{\partial \widetilde{\lambda}_{rs}}{\partial \sigma_\gamma^2}$:

For convenience, using (4.1.23) we rewrite $\widetilde{\lambda}_{rs}$ as

$$\widetilde{\lambda}_{rs} = \frac{1}{J}\sum_{j=1}^{J} q_{1j}(\beta, \sigma_\gamma^2, \phi) q_{2j}(\beta, \sigma_\gamma^2, \phi), \quad (4.2.15)$$

where

$$q_{1j}(\beta, \sigma_\gamma^2, \phi) = \frac{\exp\left[x_r'\beta + \sigma_{rr}^{*\frac{1}{2}}\left\{l_{11}\widetilde{W}_{r(s)}(j) + l_{12}\widetilde{W}_{s(r)}(j)\right\}\right]}{1 + \exp\left[x_r'\beta + \sigma_{rr}^{*\frac{1}{2}}\left\{l_{11}\widetilde{W}_{r(s)}(j) + l_{12}\widetilde{W}_{s(r)}(j)\right\}\right]}, \quad (4.2.16)$$

and

$$q_{2j}(\beta, \sigma_\gamma^2, \phi) = \frac{\exp\left[x_s'\beta + \sigma_{ss}^{*\frac{1}{2}}\left\{l_{12}\widetilde{W}_{r(s)}(j) + l_{11}\widetilde{W}_{s(r)}(j)\right\}\right]}{1 + \exp\left[x_s'\beta + \sigma_{ss}^{*\frac{1}{2}}\left\{l_{12}\widetilde{W}_{r(s)}(j) + l_{11}\widetilde{W}_{s(r)}(j)\right\}\right]}. \quad (4.2.17)$$

Note that q_{1j} in (4.2.16) and q_{2j} in (4.2.17) depend on σ_γ^2 only through $\sigma_{rr}^* = \sigma_\gamma^2[1 + (n_r - 1)\phi]$. This is because l_{11} and l_{12} involved in these functions depend on ρ_{rs}^* ((4.1.18) - (4.1.20)) which is free from σ_γ^2. For clarity we re-express σ_γ^2 as follows which is a function of the ϕ parameter only.

$$\begin{aligned}
\rho^*_{rs} &= \frac{\sigma^*_{rs}}{[\sigma^*_{rr}\sigma^*_{ss}]^{\frac{1}{2}}} \\
&= \frac{n_{rs}\left[1+(n_{rs}-1+\bar{n}_r+\bar{n}_s)\phi+\widetilde{n}_{rs}\phi\right]\sigma^2_\gamma/\sqrt{n_r n_s}}{\left[\sigma^2_\gamma(1+(n_r-1)\phi)\sigma^2_\gamma(1+(n_s-1)\phi)\right]^{\frac{1}{2}}} \\
&= \frac{n_{rs}\left[1+(n_{rs}-1+\bar{n}_r+\bar{n}_s)\phi+\widetilde{n}_{rs}\phi\right]/\sqrt{n_r n_s}}{\left[1+(n_r-1)\phi)(1+(n_s-1)\phi)\right]^{\frac{1}{2}}} \\
&= \rho^*_{rs}(n_r, n_s, n_{rs}, \bar{n}_r, \bar{n}_s, \widetilde{n}_{rs}, \phi). \qquad (4.2.18)
\end{aligned}$$

It then follows that

$$\begin{aligned}
\frac{\partial q_{1j}}{\partial \sigma^2_\gamma} &= q_{1j}\frac{[1+(n_r-1)\phi]}{2\sigma^{*\frac{1}{2}}_{rr}}\left(l_{11}\widetilde{W}_{r(s)}(j)+l_{12}\widetilde{W}_{s(r)}(j)\right) \\
&\quad - q^2_{1j}\frac{[1+(n_r-1)\phi]}{2\sigma^{*\frac{1}{2}}_{rr}}\left(l_{11}\widetilde{W}_{r(s)}(j)+l_{12}\widetilde{W}_{s(r)}(j)\right) \\
&= q_{1j}(1 - q_{1j})\frac{[1+(n_r-1)\phi]}{2\sigma^{*\frac{1}{2}}_{rr}}\left(l_{11}\widetilde{W}_{r(s)}(j)+l_{12}\widetilde{W}_{s(r)}(j)\right), \qquad (4.2.19)
\end{aligned}$$

and similarly

$$\frac{\partial q_{2j}}{\partial \sigma^2_\gamma} = q_{2j}(1 - q_{2j})\frac{[1+(n_s-1)\phi]}{2\sigma^{*\frac{1}{2}}_{rr}}\left(l_{12}\widetilde{W}_{r(s)}(j)+l_{11}\widetilde{W}_{s(r)}(j)\right). \qquad (4.2.20)$$

It then follows from (4.2.15) that

$$\frac{\partial \widetilde{\lambda}_{rs}}{\partial \sigma^2_\gamma} = \frac{1}{J}\sum_{j=1}^{J}\left[\frac{\partial q_{1l}}{\partial \sigma^2_\gamma}q_{2j} + q_{1j}\frac{\partial q_{2j}}{\partial \sigma^2_\gamma}\right], \qquad (4.2.21)$$

where $\frac{\partial q_{1j}}{\partial \sigma^2_\gamma}$ and $\frac{\partial q_{2j}}{\partial \sigma^2_\gamma}$ are given in (4.2.19) and (4.2.20) respectively. This completes the computation for the derivative required in the GQL estimating equation (4.2.10) for σ^2_γ.

4.2.4.2 Computation of $\frac{\partial \widetilde{\lambda}'}{\partial \phi}$

Next the derivative vector $\frac{\partial \widetilde{\lambda}'}{\partial \phi}$ involved in the GQL estimating equation (4.2.12) can be computed by using the derivatives $\frac{\partial \widetilde{\lambda}'_1}{\partial \phi}$ and $\frac{\partial \widetilde{\lambda}'_2}{\partial \phi}$. Further the derivative $\frac{\partial \widetilde{\lambda}'_1}{\partial \phi}$ can be computed by computing the derivatives using $\frac{\partial \widetilde{\pi}_r}{\partial \phi}$ $(r = 1, \cdots, S)$ only, where $\widetilde{\pi}_r$ is given by (4.1.8). Similarly the derivative $\frac{\partial \widetilde{\lambda}'_2}{\partial \phi}$ can be computed by using the formula for $\frac{\partial \widetilde{\lambda}_{rs}}{\partial \phi}$ from (4.1.23) for all $r \neq s, r, s = 1, \cdots, S$.

Computation of $\frac{\partial \widetilde{\pi}_r}{\partial \phi}$:

Notice that in (4.1.8), ϕ is involved only in σ^*_{rr}, by (4.0.6) which has the formula $\sigma^*_{rr} = \sigma^2_\gamma[1 + (n_r - 1)\phi]$. It then follows that

$$\frac{\partial \widetilde{\pi}_r}{\partial \phi} = \frac{1}{J}\sum_{j=1}^{J} \pi^*_r(W_{r(s)}(j))[1 - \pi^*_r(W_{r(s)}(j))] \left[(n_r - 1)\sigma^2_\gamma\right] \frac{W_{r(s)}(j)}{2\sigma^{*\frac{1}{2}}_{rr}}. \quad (4.2.22)$$

Computation of $\frac{\partial \widetilde{\lambda}_{rs}}{\partial \phi}$:

Note that q_{1j} and q_{2j} are involved in $\widetilde{\lambda}_{rs}$ in (4.2.15) contains $\sigma^*_{rr}, \sigma^*_{ss}, l_{11}$, and l_{12} which all are function of ϕ. For convenience, we compute the derivatives of these functions with respect to ϕ. That is,

$$\frac{\partial \sigma^*_{rr}}{\partial \phi} = (n_r - 1)\sigma^2_\gamma, \quad (4.2.23)$$

$$\frac{\partial \sigma^*_{ss}}{\partial \phi} = (n_s - 1)\sigma^2_\gamma. \tag{4.2.24}$$

Further

$$\begin{aligned}\frac{\partial l_{11}}{\partial \phi} &= -\frac{\rho^*_{rs}\rho^{*'}_{rs}}{\sqrt{1-\rho^{*2}_{rs}}}\sqrt{\frac{2}{1+\sqrt{1-\rho^{*2}_{rs}}}} \\ &= l'_{11} \quad \text{(say)},\end{aligned} \tag{4.2.25}$$

with

$$\begin{aligned}\rho^{*'}_{rs} &= \frac{\partial \rho^*_{rs}}{\partial \phi} \\ &= \frac{\left[n_{rs} - 1 + \bar{n}_r + \bar{n}_s + \widetilde{n}_{rs}\right]/\sqrt{n_r n_s}}{\left[(1+(n_r-1)\phi)(1+(n_s-1)\phi)\right]^{\frac{1}{2}}} \\ &\quad - \frac{n_{rs}\left[1 + (n_{rs} - 1 + \bar{n}_r + \bar{n}_s)\phi + \widetilde{n}_{rs}\phi\right]\left[(n_s-1)\sqrt{1+(n_r-1)\phi}\right]}{\sqrt{n_r n_s}(1+(n_r-1)\phi)(1+(n_s-1)\phi)} \\ &\quad - \frac{n_{rs}\left[1 + (n_{rs} - 1 + \bar{n}_r + \bar{n}_s)\phi + \widetilde{n}_{rs}\phi\right]\left[(n_r-1)\sqrt{1+(n_s-1)\phi}\right]}{\sqrt{n_r n_s}(1+(n_r-1)\phi)(1+(n_s-1)\phi)},\end{aligned} \tag{4.2.26}$$

and

$$\begin{aligned}\frac{\partial l_{12}}{\partial \phi} &= \frac{\rho^{*'}_{rs}}{2\left(1+\sqrt{1-\rho^{*2}_{rs}}\right)} + \frac{\rho^{*2}_{rs}\rho^{*'}_{rs}}{\sqrt{1-\rho^{*2}_{rs}}\left[1+\sqrt{1-\rho^{*2}_{rs}}\right]} \\ &= l'_{12} \quad \text{(say)},\end{aligned} \tag{4.2.27}$$

for which $\rho^{*'}_{rs}$ may be replaced by using (4.2.26). It then follows that

$$\begin{aligned}\frac{\partial q_{1j}}{\partial \phi} &= q_{1j}(1 - q_{1j})\left[\frac{(n_r-1)\sigma^2_\gamma}{2\sigma^{*\frac{1}{2}}_{rr}}\left(l_{11}\widetilde{W}_{r(s)}(j) + l_{12}\widetilde{W}_{s(r)}(j)\right)\right. \\ &\quad \left. + \sigma^{*\frac{1}{2}}_{rr}\left(l'_{11}\widetilde{W}_{r(s)}(j) + l'_{12}\widetilde{W}_{s(r)}(j)\right)\right],\end{aligned} \tag{4.2.28}$$

and similarly

$$\frac{\partial q_{2j}}{\partial \phi} = q_{2j}(1 - q_{2j}) \left[\frac{(n_s - 1)\sigma_\gamma^2}{2\sigma_{ss}^{*\frac{1}{2}}} \left(l_{12}\widetilde{W}_{r(s)}(j) + l_{11}\widetilde{W}_{s(r)}(j) \right) + \sigma_{ss}^{*\frac{1}{2}} \left(l'_{12}\widetilde{W}_{r(s)}(j) + l'_{11}\widetilde{W}_{s(r)}(j) \right) \right]. \quad (4.2.29)$$

It then follows from (4.2.15) that

$$\frac{\partial \widetilde{\lambda}_{rs}}{\partial \phi} = \frac{1}{J} \sum_{j=1}^{J} \left[\frac{\partial q_{1j}}{\partial \phi} q_{2j} + q_{1j} \frac{\partial q_{2j}}{\partial \phi} \right] \quad (4.2.30)$$

where $\frac{\partial q_{1j}}{\partial \phi}$ and $\frac{\partial q_{2j}}{\partial \phi}$ are given in (4.2.28) and (4.2.29) respectively. This completes the computation for the derivative required in the GQL estimating equations (4.2.12) for ϕ.

4.2.5 Construction of the Covariance Matrix Ω

We write the covariance matrix $\Omega = \text{cov}(U)$ as

$$\Omega = \begin{pmatrix} \widetilde{\Sigma} & P \\ P' & M \end{pmatrix}, \quad (4.2.31)$$

where $\widetilde{\Sigma} = \text{var}(Y)$, $P = \text{cov}(U_1, U_2)$ and $M = \text{cov}(U_2)$. For clarity, we write the formulas for these matrices in the following sub sections.

4.2.5.1 Construction of $\widetilde{\Sigma}$

Recall that (4.1.9) for $r = 1, \cdots, S$, the diagonal elements of the $\widetilde{\Sigma}$ matrix is given by

$$\widetilde{\sigma}_{rr} = \text{var}(Y_r) = \widetilde{\pi}_r(1 - \widetilde{\pi}_r). \tag{4.2.32}$$

Similarly by using (4.1.15), for $r \neq s$, the off diagonal elements of the $\widetilde{\Sigma}$ matrix is given by

$$\widetilde{\sigma}_{rs} = \text{cov}(Y_r, Y_s) = \widetilde{\lambda}_{rs} - \widetilde{\pi}_r\widetilde{\pi}_s, \tag{4.2.33}$$

where $\widetilde{\pi}_r$ $(r = 1, \cdots, S)$ in both (4.2.32) and (4.2.33) is computed by (4.1.8) and $\widetilde{\lambda}_{rs}$ in (4.2.33) is computed by (4.1.13).

4.2.5.2 Construction of P

The construction of the P matrix requires the components of $\text{cov}(Y_r, Y_sY_{s+1})$ for all values of r and s.

Case 1: For $r = s$

$$\begin{aligned}
\text{cov}(Y_r, Y_rY_{r+1}) &= E\left(Y_r^2Y_{r+1}\right) - \widetilde{\pi}_r\widetilde{\lambda}_{r,r+1} \\
&= E(Y_rY_{r+1}) - \widetilde{\pi}_r\widetilde{\lambda}_{r,r+1} \\
&= \widetilde{\lambda}_{r,r+1} - \widetilde{\pi}_r\widetilde{\lambda}_{r,r+1} \\
&= \widetilde{\lambda}_{r,r+1}(1 - \widetilde{\pi}_r).
\end{aligned} \tag{4.2.34}$$

Case 2: For $r \neq s$, one requires the computation of the distinct third order moments given by

$$\begin{aligned} \text{cov}(Y_r, Y_s Y_{s+1}) &= E(Y_r Y_s Y_{s+1}) - E(Y_r)E(Y_s Y_{s+1}) \\ &= \widetilde{\delta}_{rs,s+1} - \widetilde{\pi}_r \widetilde{\lambda}_{s,s+1} \quad \text{(say)}. \end{aligned} \tag{4.2.35}$$

Note that the exact computation for the third order moments $\widetilde{\delta}_{rs,s+1}$, similar to but different than (4.1.23), requires the generation of three correlated standardized random effects. Hence this approach would be naturally complicated . However, as the consistency of the estimator does not require the exact covariance matrix Ω, some authors such as Prentice and Zhao (1991) [see also Sutradhar (2011), section 8.3.1] have used a normal approximation to the binary data where binary responses are treated to be normal but with correct means, variances and covariances. We follow this approach and derive $\widetilde{\delta}_{rs,s+1}$ from

$$E(Y_r - \widetilde{\pi}_r)(Y_s - \widetilde{\pi}_s)(Y_{s+1} - \widetilde{\pi}_{s+1}) = 0.$$

Thus,

$$\begin{aligned} \widetilde{\delta}_{rs,s+1} &= E(Y_r Y_s Y_{s+1}) \\ &= \widetilde{\sigma}_{rs}\widetilde{\pi}_{s+1} + \widetilde{\sigma}_{r,s+1}\widetilde{\pi}_s + \widetilde{\sigma}_{s,s+1}\widetilde{\pi}_r - 2\widetilde{\pi}_r\widetilde{\pi}_s\widetilde{\pi}_{s+1}, \end{aligned} \tag{4.2.36}$$

where $\widetilde{\pi}_r$ and $\widetilde{\sigma}_{rs}$, for example, are correct means and covariances for the binary responses. This completes the construction of $S \times S(S-1)/2$ dimension of P matrix.

4.2.5.3 Construction of M

The computation of the elements of the $S(S+1)/2 \times S(S+1)/2$ matrix M requires the computation of $\mathrm{cov}(Y_rY_{r+1}, Y_sY_{s+1})$ for all $r, s = 1, \cdots, S-1$.

Case 1: For $r = s$, we obtain

$$\begin{aligned}
\mathrm{cov}(Y_rY_{r+1}, Y_rY_{r+1}) &= E(Y_r^2Y_{r+1}^2) - E(Y_rY_{r+1})E(Y_sY_{s+1}) \\
&= \widetilde{\lambda}_{r,r+1} - \widetilde{\lambda}^2_{r,r+1} \\
&= \widetilde{\lambda}_{r,r+1}(1 - \widetilde{\lambda}_{r,r+1}) \qquad (4.2.37)
\end{aligned}$$

Case 2: For $r \neq s$, we compute the fourth order moments given by

$$\begin{aligned}
\mathrm{cov}(Y_rY_{r+1}, Y_sY_{s+1}) &= E(Y_rY_{r+1}Y_sY_{s+1}) - E(Y_rY_{r+1})E(Y_sY_{s+1}) \\
&= \widetilde{\xi}_{r,r+1,s,s+1} - \widetilde{\lambda}_{r,r+1}\widetilde{\lambda}_{s,s+1} \quad \text{(say)}. \qquad (4.2.38)
\end{aligned}$$

Under the normality assumption, similar to the approach of third moments, we follow Prentice and Zhao (1991) [see also Sutradhar (2011, section 8.3.1)] and derive $\widetilde{\xi}_{r,r+1,s,s+1}$ from

$$E(Y_r - \widetilde{\pi}_r)(Y_s - \widetilde{\pi}_s)(Y_t - \widetilde{\pi}_t)(Y_u - \widetilde{\pi}_u) = \widetilde{\sigma}_{rs}\widetilde{\sigma}_{tu} + \widetilde{\sigma}_{rt}\widetilde{\sigma}_{su} + \widetilde{\sigma}_{ru}\widetilde{\sigma}_{st}. \qquad (4.2.39)$$

Thus, by using (4.2.39), we then obtain the fourth order product moment under normality as

$$\begin{aligned}
\widetilde{\xi}_{r,r+1,s,s+1} &= E(Y_r Y_{r+1} Y_s Y_{s+1}) \\
&= \widetilde{\sigma}_{r,r+1}\widetilde{\sigma}_{s,s+1} + \widetilde{\sigma}_{rs}\widetilde{\sigma}_{r+1,s+1} + \widetilde{\sigma}_{r,s+1}\widetilde{\sigma}_{r+1,s} \\
&\quad + \widetilde{\delta}_{r,r+1,s}\widetilde{\pi}_{s+1} + \widetilde{\delta}_{r,r+1,s+1}\widetilde{\pi}_s + \widetilde{\delta}_{r+1,s,s+1}\widetilde{\pi}_r \\
&\quad - \widetilde{\sigma}_{r,r+1}\widetilde{\pi}_s\widetilde{\pi}_{s+1} - \widetilde{\sigma}_{s,s+1}\widetilde{\pi}_r\widetilde{\pi}_{r+1} - \widetilde{\sigma}_{rs}\widetilde{\pi}_{r+1}\widetilde{\pi}_{s+1} - \widetilde{\sigma}_{r+1,s+1}\widetilde{\pi}_r\widetilde{\pi}_s \\
&\quad -\widetilde{\sigma}_{r,s+1}\widetilde{\pi}_{r+1}\widetilde{\pi}_s - \widetilde{\sigma}_{r+1,s}\widetilde{\pi}_r\widetilde{\pi}_{s+1} + 3\widetilde{\pi}_r\widetilde{\pi}_{r+1}\widetilde{\pi}_s\widetilde{\pi}_{s+1} \qquad (4.2.40)
\end{aligned}$$

This completes the construction of the $S(S+1)/2 \times S(S+1)/2$ matrix M.

Chapter 5

Concluding Remarks

In spatial regression setup, the responses from the neighboring locations are bound to be correlated. It is important to take such correlations into account while estimating the regression effects of the covariates on the responses from the locations. Our literature review indicated that the existing studies modeled the spatial correlations mainly through temporal type (time series oriented) dynamic relationship. In this thesis we proposed a unified random effects approach to model the spatial correlations. The correlation models are developed in such way that even if the random effects from different locations are independent, the responses from neighboring locations still would be correlated. Under specialized linear sequence of spatial locations, we have examined the performance of the well-known MM and ML approaches in estimating the regression effects and variance of the random effects. Note that in this problem, correlations were mainly functions of the number of members n_r (in the r^{th} family) and the number of common members n_{rs} (between r^{th} and s^{th} family). It was found that the estimates were in complete agreement with the true values of the parameters.

When random effects are pairwise correlated (equi-correlated), we have developed a scheme how they can be generated and incorporated in the correlation model for the responses. We have generalized the correlation model for linear data to the binary data case. As far as the inference is concerned, all necessary computations are shown in order to develop a consistent and efficient GQL approach.

Note that the proposed new correlation models may be applied for efficient real life data analysis both for linear and binary cases. Furthermore, it would be useful to blend this spatial correlation modeling concept with available temporal correlation model for temporal data, in order to develop familial longitiudinal type combined correlation models. However, these are beyond the scope of the present thesis.

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