Spatial automatic subgroup analysis for areal data with repeated measures

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Abstract

We consider the subgroup analysis problem for spatial areal data with repeated measures. To take into account spatial data structures, we propose to use a class of spatially-weighted concave pairwise fusion method which minimizes the objective function subject to a weighted pairwise penalty, referred as Spatial automatic Subgroup analysis (SaSa). The penalty is imposed on all pairs of observations, with the location specific weight being chosen for each pair based on their corresponding spatial information. The alternating direction method of multiplier algorithm (ADMM) is applied to obtain the estimates. We show that the oracle estimator based on weighted least squares is a local minimizer of the objective function with probability approaching 1 under some conditions, which also indicates the clustering consistency properties. In simulation studies, we demonstrate the performances of the proposed method equipped with different weights in terms of their accuracy for estimating the number of subgroups. The results suggest that spatial information can enhance subgroup analysis in certain challenging situations when the minimal group difference is small or the number of repeated measures is small. The proposed method is then applied to find the relationship between two surveys, which can provide spatially interpretable groups.

key words: Areal data; Linear regression; Penalization; Repeated measures; Spatial clustering; Subgroup analysis

1 Introduction

Spatial clustering or spatial boundaries detection is critically important in disease mapping, spatial epidemiology and population genetics (Hegarty and Barry, 2008; Reich and...
In literature, there are a variety of methods for spatial data clustering. For example, Lu and Carlin (2005) and Lu et al. (2007) considered the areal boundary detection using a Bayesian hierarchical model based on the conditional autoregressive model (Banerjee et al., 2014). The boundaries were determined by the posterior distribution of the corresponding spatial process or spatial weights. These boundary detection methods focused on clustering of observations instead of regression coefficients. Li et al. (2011) proposed a method based on Bayesian information criteria (BIC) combined with spatial neighborhood information for boundary detection in spatial areal data. Li et al. (2015) used the Dirichlet process and false discovery rate to detect boundaries under a hierarchical model setting. These models detected the boundaries through modeling the spatial random effect with the same regression coefficients for all areas. The Dirichlet process was also involved in modeling the spatial dependence in genetics data to identify homogeneous groups without considering a regression model (Reich and Bondell, 2011). Hegarty and Barry (2008) applied the product partition model (Hartigan, 1990) in a disease mapping problem without considering covariates and spatial information. Page and Quintana (2016) proposed the spatial product partition model with covariates, which put priors on the partitions according to the spatial locations of observations. All the above methods didn’t provide theoretical results.

For non-spatial data clustering, there are some methods which tackle the problem through solving an optimization problem. In particular, Chi and Lange (2015) developed a method for the convex clustering problem through the alternating direction method of multiplier algorithm (ADMM) (Boyd et al., 2011) with pairwise $L_p(p \geq 1)$ penalty. Nonnegative weights are considered to reduce bias for pairwise penalties. Fan and Guan (2018) considered a clustering problem with $l_0$ penalty on graphs. These two methods are developed for clustering based on observations. Besides clustering observations, there is another class of methods to identify clusters or homogeneous groups based on regression coefficients. Ma and Huang (2017) and Ma et al. (2018) extended the problem to linear regression settings and used the smoothly clipped absolute deviation (SCAD) penalty (Fan and Li, 2001) and the minimax concave penalty (MCP) (Zhang, 2010), where theoretical properties of the estimators were also studied.

In spatial data analysis, observations near each other could share similar patterns, so the spatial dependence information should be considered in models to find homogeneous groups. However, there are some unique challenges in the problem of spatial clustering. First, how to properly utilize spatial information when detecting clusters? Second, it is difficult to estimate the number of clusters (or subgroups) and cluster memberships consistently. Despite their effective performances in real applications, most of existing spatial data methods did not provide the theoretical results of estimators. In this article, we develop and study the SaSa algorithm, which is a class of spatially-regulated clustering methods, to tackle these challenges and achieve spatial clustering consistency in the context of linear regression models. In particular, the new method can identify subgroups based on the similarities of regression coefficients for spatial areal data with repeated measures. We impose the weighted pairwise concave penalty on differences...
among group (cluster) regression coefficients, where the weights are constructed for each pair based on their spatial relationship, which are location specific. We consider a number of different pairwise weights and study them numerically and theoretically. In theory, we show that the oracle estimator based on weighted least squares is a local minimizer of the objective function with probability approaching 1 under some conditions, which indicates that the number of clusters can be estimated consistently. Our numerical examples suggest that, the number of clusters and the group structure can be recovered with high probability, and the spatial information can help in spatial subgroup analysis when the minimal group difference is small or the number of repeated measures is small.

The article is organized as follows. In Section 2, we describe the Spatial automatic Subgroup analysis (SaSa) model and the corresponding ADMM algorithm. In Section 3, we establish theoretical properties of the proposed SaSa estimator. The simulation study is conducted in Section 4 under several scenarios to show performances of the proposed estimator. We use an example to illustrate our proposed estimator in real-data applications in Section 5. Finally, some discussions are given in Section 6.

2 The SaSa model and the algorithm

In Section 2.1, the SaSa model and the corresponding objective function are introduced. In Section 2.2, we study the computational issue and describe the ADMM algorithm to optimize the objective function.

2.1 The model with repeated measures

Assume our spatial data consist of multiple measurements at each location or subject. Let $y_{ih}$ be the $h$th response for the $i$th subject observed at location $s_i$, where $i = 1, \ldots, n$, $h = 1, \ldots, n_i$. Based on their effects on the response variable, the covariates can be divided into two categories: “global” covariates which have common effects on the response across all the locations, and “local” covariates which have location-specific effects on the response. To reflect this, let $z_{ih}$ and $x_{ih}$ be the corresponding covariate vectors with dimension $q$ and $p$ respectively, where $z_{ih}$’s are “global” covariates which have common linear effects to the response across all the locations, while $x_{ih}$’s are “local” covariates which have location-specific linear effects on the response. We consider the following linear regression model

$$y_{ih} = z_{ih}'\eta + x_{ih}'\beta_i + \epsilon_{ih},$$

where $\eta$ represents the vector of common regression coefficients shared by global effects, $\beta_i$’s are location-specific regression coefficients, and $\epsilon_{ih}$’s are i.i.d random errors with $E(\epsilon_{ih}) = 0$ and $Var(\epsilon_{ih}) = \sigma^2$. Furthermore, some locations may have same or similar location-specific effects, grouping locations of same location-specific effects can help to achieve dimension reduction and improve model prediction accuracy. Assume the $n$ location-specific effects belong to $K$ mutually exclusive subgroups: the locations with a common $\beta_i$ belong to the same group. Denote the corresponding partition of $\{1, \ldots, n\}$
as \( G = \{ G_1, \ldots, G_K \} \), where the index set \( G_k \) contains all the locations belonging to the group \( k \) for \( k = 1, \ldots, K \). For convenience, denote the regression coefficients associated with \( G_k \) as \( \alpha_k \). In practice, since neither \( K \) nor the partition \( G_k \)'s are known, the goal is to use the observed data \( \{(y_{ih}, z_{ih}, x_{ih})\} \) to construct the estimator \( \hat{K} \) and the partition \( \hat{G} = \{ \hat{G}_1, \ldots, \hat{G}_K \} \), where \( \hat{G}_k = \{ i : \hat{\beta}_i = \hat{\alpha}_k, 1 \leq i \leq n \} \).

To achieve this goal, we use the following optimization problem: minimize the weighted least squares objective function subject to a spatially-weighted pairwise penalty

\[
Q_n(\eta, \beta; \lambda, \psi) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{n_i} \sum_{h=1}^{n_i} (y_{ih} - z_{ih}^T \eta - x_{ih}^T \beta)^2 + \sum_{1 \leq i < j \leq n} p_\gamma(\|\beta_i - \beta_j\|, c_{ij} \lambda),
\]

where \( \eta = (\eta_1, \ldots, \eta_q)^T, \beta = (\beta_1^T, \ldots, \beta_n^T)^T, || \cdot || \) denotes the Euclidean norm, \( p_\gamma(\cdot, \lambda) \) is a penalty function imposed on all distinct pairs. In the penalty function, \( \lambda \geq 0 \) is a tuning parameter, \( \gamma > 0 \) is a built-in constant in the penalty function, and different weights \( c_{ij} \)'s are assigned to different pairs of locations \( s_i \) and \( s_j \) for any \( 1 \leq i < j \leq n \). One popular choice of penalty is the \( L_1 \) penalty (lasso) (Tibshirani, 1996) with the form \( p_\gamma(t, \lambda) = \lambda |t| \). Since \( L_1 \) penalty tends to produce too many groups as shown in Ma and Huang (2017), we consider the SCAD penalty, which is defined as

\[
p_\gamma(t, \lambda) = \lambda \int_0^{|t|} \min\{1, (\gamma - x/\lambda)_+ / (\gamma - 1)\} \, dx.
\]

Here we treat \( \gamma \) as a fixed value as in Fan and Li (2001), Zhang (2010) and Ma et al. (2018).

In (2), the values weights \( c_{ij} \) are crucial, as they control the number of subgroups and grouping results. The pairs \( \| \beta_i - \beta_j \| \) with larger weights \( c_{ij} \lambda \) are shrunk together more than those pairs with smaller weights. For spatial data, reasonable choices of \( c_{ij} \) should take into account two factors: locations with closer \( \beta \) values are more grouped together, and locations closer to each other are more likely to form a subgroup as they typically have similar trends. Since the true values of \( \beta \) are not available, we use their estimators \( \hat{\beta} \) as the surrogates. For example, we can define the weights \( c_{ij} \) as

\[
c_{ij} = \exp\left(-\psi \|s_i - s_j\| \cdot \|\hat{\beta}_i - \hat{\beta}_j\|\right),
\]

where \( \hat{\beta}_i \) is an initial estimate of \( \beta_i \), and \( \psi \) is a scale parameter to control magnitudes of the weights. In areal data, we suggest three different ways of taking into spatial information in the data to construct the weights.

(i) using both spatial and regression coefficients information:

\[
c_{ij} = \exp\left(\psi (1 - a_{ij}) \cdot \|\hat{\beta}_i - \hat{\beta}_j\|\right),
\]

where \( a_{ij} \) is the neighbor order between location \( s_i \) and location \( s_j \), which means that if \( i \) and \( j \) are neighbors, \( a_{ij} = 1 \). If \( i \) and \( j \) are not neighbors, but they have at least one same neighbor, \( a_{ij} = 2 \). Similarly, we can have all the neighborhood order for all
subjects or locations.

(ii) using regression coefficients information only:

\[ c_{ij} = \exp \left( -\psi \| \tilde{\beta}_i - \tilde{\beta}_j \| \right). \]  

(iii) using spatial information only:

\[ c_{ij} = \exp \left( \psi (1 - a_{ij}) \right). \]  

Weights in (4) and (5) both includes the regression coefficients, which would depend on the accuracy of \( \tilde{\beta}_i \). If the number of repeated measures is not large, the values of \( \tilde{\beta}_i \) will not show the real relationship between different locations, which would lead to very bad weights. The phenomenon can be observed in the simulation study. The weights we use here are three special cases which use the information of either regression coefficients or the spatial neighborhood orders. Definitely, there are other ways to construct weights, such as using distance to borrow the spatial information. At least the weights satisfy condition (C4) in Section 3, the theoretical results will hold under other conditions. For example, the weights in (5) will satisfy (C4) automatically if \( \tilde{\beta}_i \)'s are consistent estimators. That is, besides the condition (C4), there are no other conditions about the format of the weight function.

### 2.2 The SaSa algorithm

In this section, we describe the ADMM algorithm to solve (2) in Section 2.1. The algorithm shares the same spirit as Ma and Huang's (2017), where a non-weighted penalty is used in non-spatial settings without repeated measures.

There are two tuning parameters, \( \lambda \) and \( \psi \), in the proposed method. We choose them adaptively using some tuning procedures discussed at the end of this section. For now, we fix them and present the computational algorithm for solving (2). Denote the solution as

\[ (\hat{\eta}, \hat{\beta}) = \arg\min_{\eta \in \mathbb{R}^q, \beta \in \mathbb{R}^{np}} Q_n (\eta, \beta, \lambda, \psi). \]  

First, we introduce the slack variables for all the pairs \((i, j)\) \( \delta_{ij} = \beta_i - \beta_j \), for \( 1 \leq i < j \leq n \). Then the problem is equivalent to minimizing the following objective function with regard to \((\eta, \beta, \delta)\),

\[
\min_{\eta, \beta, \delta} L_0 (\eta, \beta, \delta) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{n_i} \sum_{h=1}^{n_i} \left( y_{ih} - z_{ih}^T \eta - x_{ih}^T \beta_i \right)^2 + \sum_{1 \leq i < j \leq n} p_\gamma (\| \delta_{ij} \|, c_{ij} \lambda),
\]

subject to \( \beta_i - \beta_j - \delta_{ij} = 0, \ 1 \leq i < j \leq n \),

where \( \delta = (\delta_{ij}^T, 1 \leq i < j \leq n)^T \). To handle the equation constraints in the optimization problem, we introduce the augmented Lagrangian

\[
L (\eta, \beta, \delta, v) = L_0 (\eta, \beta, \delta) + \sum_{i < j} \langle v_{ij}, \beta_i - \beta_j - \delta_{ij} \rangle + \frac{\psi}{2} \sum_{i < j} \| \beta_i - \beta_j - \delta_{ij} \|^2 ,
\]
where \( v = (v_{ij}^T, 1 \leq i < j \leq n)^T \) are Lagrange multipliers and \( \vartheta > 0 \) is the penalty parameter.

To solve the problem, we use an iterative algorithm which updates \( \boldsymbol{\beta}, \eta, \delta, v \) sequentially, one at a time. At the \((m+1)\)th iteration, given their current values \((\boldsymbol{\beta}^{(m)}, \eta^{(m)}, \delta^{(m)}, v^{(m)})\), the updates of \( \eta, \delta, \beta, v \) are

\[
\begin{align*}
(\eta^{(m+1)}, \beta^{(m+1)}) &= \arg\min_{\eta, \beta} L(\eta, \beta, \delta^{(m)}, v^{(m)}), \\
\delta^{(m+1)} &= \arg\min_{\delta} L(\eta^{(m+1)}, \beta^{(m+1)}, \delta, v^{(m)}), \\
v_{ij}^{(m+1)} &= v_{ij}^{(m)} + \vartheta \left( \beta_{ij}^{(m+1)} - \beta_{ij}^{(m)} - \delta_{ij}^{(m+1)} \right).
\end{align*}
\] (8)

To update \( \eta \) and \( \beta \), we minimize the following objective function

\[
f(\beta, \eta) = \| \Omega^{1/2} (y - Z\eta - X\beta) \|^2 + \vartheta \| A\beta - \delta^{(m)} + \vartheta^{-1} v^{(m)} \|^2,
\]

where \( \eta = (\eta_1, \ldots, \eta_{n-1})^T \), \( Z = (z_{11}, \ldots, z_{1n}, \ldots, z_{n1}, \ldots, z_{nn})^T \), \( X = \text{diag}(x_1, \ldots, x_n) \) with \( x_i = (x_{i1}, \ldots, x_{in})^T \), \( \Omega = \text{diag}(1/n_1, \ldots, 1/n_n) \) and \( A = D \otimes I_p \) with an \([n(n-1)/2] \times n\) matrix \( D = \{ (e_i - e_j) \}^T \), where \( e_i \) is an \( n \times 1 \) vector with \( i \)th element 1 and other elements 0. Then the solutions for \( \beta \) and \( \eta \) are

\[
\begin{align*}
\beta^{(m+1)} &= (X^T Q_{Z,\Omega} X + \vartheta A^T A)^{-1} \left[ X^T Q_{Z,\Omega} y + \vartheta \text{vec} \left( \left( \Delta^{(m)} - \vartheta^{-1} \gamma^{(m)} \right) D \right) \right], \\
\eta^{(m+1)} &= (Z^T \Omega Z)^{-1} Z^T \Omega \left( y - X \beta^{(m+1)} \right),
\end{align*}
\] (9)

where \( \Delta^{(m)} = \left( \delta_{ij}^{(m)} \right)_{i < j} \) and \( \gamma^{(m)} = \left( v_{ij}^{(m)} \right)_{i < j} \) are the updates of the \( \delta \) and \( v \) respectively.

To update \( \delta_{ij} \)'s componentwisely, it is equivalent to minimize the following objective function

\[
\frac{\vartheta}{2} \| S_{ij}^{(m+1)} - \delta_{ij} \|^2 + p_\gamma(\| \delta_{ij} \|, c_{ij} \gamma),
\]

where \( S_{ij}^{(m+1)} = (\beta_{ij}^{(m+1)} - \beta_{ij}^{(m+1)}) + \vartheta^{-1} v_{ij}^{(m)} \). The solution based on SCAD penalty has a closed-form solution as

\[
\delta_{ij}^{(m+1)} = \begin{cases} 
\frac{S_{ij}^{(m+1)} - \lambda c_{ij} / \vartheta}{\lambda c_{ij} / \vartheta} & \text{if } \| S_{ij}^{(m+1)} \| \leq \lambda c_{ij} + \lambda c_{ij} / \vartheta, \\
\frac{S_{ij}^{(m+1)} - \gamma \lambda c_{ij} / ((\gamma - 1) \vartheta)}{\lambda c_{ij} / ((\gamma - 1) \vartheta)} & \text{if } \lambda c_{ij} + \lambda c_{ij} / \vartheta < \| S_{ij}^{(m+1)} \| \leq \gamma \lambda c_{ij}, \\
\frac{S_{ij}^{(m+1)}}{\lambda c_{ij} / (\gamma - 1) \vartheta} & \text{if } \| S_{ij}^{(m+1)} \| > \gamma \lambda c_{ij},
\end{cases}
\] (10)
where \( \gamma > c_{ij} + c_{ij}/\vartheta \) and \( S(w, t) = (1 - t/\|w\|)_+ w \), and \((t)_+ = t \) if \( t > 0 \), 0 otherwise.

In summary, the computational algorithm can be described as follows.

**Algorithm: ADMM algorithm**

**Require:** Initialize \( \beta^{(0)} \), \( \delta^{(0)} \) and \( v^{(0)} \).

1: for \( m = 0, 1, 2, \ldots \) do
2: Update \( \beta \) by (9).
3: Update \( \eta \) by (10).
4: Update \( \delta \) by (11).
5: Update \( v \) by (8).
6: if convergence criterion is met then
7: Stop and get the estimates
8: else
9: \( m = m + 1 \)
10: end if
11: end for

If the size of \( n_i \) is reasonable, such as 10 or larger, we construct the initial values \( \tilde{\beta}^{(0)} \) by fitting a linear regression model \( y_{ih} = z_{ih}^T \eta + x_{ih}^T \beta_i + \epsilon_{ih} \) for each \( i = 1, \ldots, n \).

Then, set \( \delta_{ij}^{(0)} = \beta_i^{(0)} - \beta_j^{(0)} \) and \( v^{(0)} = 0 \). If \( n_i = 1 \) or small, the initial values can be set using the procedure in Ma et al. (2018). They used a ridge fusion criterion with a small value of the tuning parameter, then the initial group structure was obtained by assigning objects into \( K^* \) (a given value) groups by ranking the estimated \( \hat{\beta}_i \).

If \( \hat{\delta}_{ij} = 0 \), then the location \( i \) and \( j \) belong to the same group. Thus, we can obtain the corresponding estimated partition \( \hat{G} \) and the estimated number of groups \( \hat{K}(\lambda, \psi) \).

For each group, its group-specific parameter vector is estimated as \( \hat{\alpha}_k = 1/|\hat{G}_k| \sum_{i \in \hat{G}_k} \hat{\beta}_i \) for \( k = 1, \ldots, \hat{K} \).

**Remark 1.** If there are no global covariates, the model is simplified as \( y_{ih} = x_{ih}^T \beta_i + \epsilon_{ih} \). The algorithm will be simplified, that is, \( QZ, \Omega \) will become \( \Omega \). The model we use in the application is the simplified model.

**Remark 2.** The convergence criterion used is the same as Ma and Huang (2017), which is based on the primal residual \( r^{(m+1)} = A\beta^{(m+1)} - \delta^{(m+1)} \). The algorithm is stopped if \( \|r^{(m+1)}\| < \varepsilon \), where \( \varepsilon \) is a small positive value.

We need to select two tuning parameters, \( \lambda \) and \( \psi \), in the SaSa algorithm. In this paper, we use the modified Bayes Information Criterion (BIC) (Wang et al., 2007) to determine the best tuning parameters adaptively from the data. In particular, we have

\[
\text{BIC}(\lambda, \psi) = \log \left[ \frac{1}{n} \sum_{i=1}^{n} \frac{1}{n_i} \left( y_{ih} - z_{ih}^T \hat{\eta}(\lambda, \psi) - x_{ih}^T \hat{\beta}_i(\lambda, \psi) \right)^2 \right] + C_n \frac{\log n}{n} \left( \hat{K}(\lambda, \psi)p + q \right),
\]

(12)
where \( C_n \) is a positive number which can depend on \( n \). Here we use \( C_n = c_0 \log (\log (np + q)) \) following Ma and Huang (2017) with \( c_0 = 0.2 \). To select \( \psi \), we select the best value from a set of candidate values, such as 0.1, 0.5, 1, 3. For each given \( \psi \), we use the warm start and continuation strategy as in Ma et al. (2018) to select tuning parameter \( \lambda \). A grid of \( \lambda \) is predefined within \([\lambda_{\text{min}}, \lambda_{\text{max}}]\). For each \( \lambda \), the initial values are the estimated values from the previous estimation. Denote the selected tuning parameters as \( \hat{\lambda} \) and \( \hat{\psi} \).

Correspondingly, the estimated group number is \( \hat{K}(\hat{\lambda}, \hat{\psi}) \), and the estimated regression coefficients are \( \hat{\beta} \) and \( \hat{\eta} \).

### 3 Theoretical properties

In this section, we study theoretical properties of the proposed SaSa estimator.

Assume \( G_k \)'s are the true partition of location-specific regression coefficients. Let \( |G_k| \) be the number of subjects in group \( G_k \) for \( k = 1, \ldots, K \), \( |G_{\text{min}}| \) and \( |G_{\text{max}}| \) be the minimum and maximum group sizes, respectively. Let \( \tilde{W} \) be an \( n \times K \) matrix with element \( w_{ik} \) and \( w_{ik} = 1 \) if \( i \in G_k \), \( w_{ik} = 0 \), otherwise. Denote \( W = \tilde{W} \otimes I_p \), which is an \( np \times Kp \) matrix and \( U = (\mathbf{Z}, XW) \). Define \( M_k = \{ \beta \in \mathbb{R}^{np} : \beta_i = \beta_j \text{ for } i, j \in G_k, \, 1 \leq k \leq K \} \). Using these notations, we can then express \( \beta \) as \( \beta = W\alpha \) if \( \beta \in M_k \), where \( \alpha = (\alpha_1^T, \ldots, \alpha_K^T)^T \). For any positive numbers, \( x_n \) and \( y_n \), \( x_n \gg y_n \) means that \( x_n^{-1}y_n = o(1) \). Define the scaled penalty function by

\[
\rho_\gamma(t) = \lambda^{-1}p_\gamma(t, \lambda).
\] (13)

Below are our assumptions, where (C1) and (C3) follow those in Ma et al. (2018).

(C1) The function \( \rho_\gamma(t) \) is symmetric, non-decreasing, and concave on \([0, \infty)\). It is constant for \( t \geq a\lambda \) for some constant \( a > 0 \), and \( \rho_\gamma(0) = 0 \). Also, \( \rho'(t) \) exists and is continuous except for a finite number values of \( t \) and \( \rho'(0+) = 1 \).

(C2) There exist finite positive constants \( M_1, M_2, M_3 > 0 \) such that \( |x_{ih,j}| \leq M_1 \), \( |z_{ih,j}| \leq M_1 \) for \( j = 1, \ldots, n_i \) and \( i = 1, \ldots, n \) and \( M_2 \leq \max_i n_i / \min_i n_i \leq M_3 \). Also, assume that \( \lambda_{\text{min}}(\mathbf{U}^T\Omega\mathbf{U}) \geq C_1 |G_{\text{min}}|, \quad \lambda_{\text{max}}(\mathbf{U}^T\Omega\mathbf{U}) \leq C_1 n \) for some constants \( 0 < C_1 < \infty \) and \( 0 < C_1' < \infty \), where \( \lambda_{\text{min}} \) and \( \lambda_{\text{max}} \) are the corresponding minimum and maximum eigenvalues respectively. In addition, assume that \( \sup_i \|x_{ih}\| \leq C_2\sqrt{p} \) and \( \sup_i \|z_{ih}\| \leq C_3\sqrt{q} \) for some constants \( 0 < C_2 < \infty \) and \( 0 < C_3 < \infty \).

(C3) The random error vector \( \mathbf{e} = (\epsilon_{11}, \ldots, \epsilon_{1n_1}, \epsilon_{21}, \ldots, \epsilon_{2n_2}, \ldots, \epsilon_{n1}, \ldots, \epsilon_{nn_n})^T \) has sub-Gaussian tails such that \( P(\|a^T\mathbf{e}\| > \|a\| x) \leq 2 \exp(-c_1 x^2) \) for any vector \( a \in \mathbb{R}^n \) and \( x > 0 \), where \( 0 < c_1 < \infty \) and \( m = \sum_{i=1}^n n_i \).

(C4) The pairwise weights \( c_{ij} \)'s are bounded away from zero if \( i \) and \( j \) are in the same group.
Conditions (C1) and (C3) are commonly used in high-dimensional penalized regression problems, which are also used in Ma et al. (2018). Condition (C2) is also similar to the condition mentioned in Ma et al. (2018), also includes the bounded conditions for covariates, which are used in Huang et al. (2004). In general, if the weights functions are not only defined on a finite support, \( c_{ij} \)'s will satisfy condition (C4).

First, we establish the properties of the oracle estimator, which is defined as the weighted least squares estimator assuming that the underlying group structure is known. Specifically, the oracle estimator of \((\eta, \alpha)\) is

\[
\begin{align*}
(\hat{\eta}^{\text{or}}, \hat{\alpha}^{\text{or}}) = & \arg \min_{\eta \in \mathbb{R}^q, \alpha \in \mathbb{R}^{Kp}} \frac{1}{2} \left\| \Omega^{1/2} (y - Z\eta - XW\alpha) \right\|^2 \\
= & \left( U^T \Omega \right)^{-1} U^T \Omega y.
\end{align*}
\]

(14)

And the corresponding oracle estimator of \( \beta \) is \( \hat{\beta}^{\text{or}} = W \hat{\alpha}^{\text{or}} \). Let \( \alpha^0_k \) be the true coefficient vector for group \( k, k = 1, \ldots, K \) and \( \alpha^0 = ((\alpha^0_1)^T, \ldots, (\alpha^0_K)^T)^T \), and let \( \eta^0 \) be the true common coefficient vector. The following theorem shows the properties of the oracle estimator.

**Theorem 1.** Suppose

\[
|G_{\text{min}}| \gg (q + Kp)^{1/2} \max \left( \sqrt{\frac{n}{\min_i n_i}} \log n, (q + Kp)^{1/2} \right).
\]

Under conditions (C1)-(C3), \( q = o(n) \) and \( Kp = o(n) \), we have with probability at least \( 1 - 2(q + Kp)n^{-1} \),

\[
\left\| \begin{pmatrix} \hat{\eta}^{\text{or}} - \eta^0 \\ \hat{\alpha}^{\text{or}} - \alpha^0 \end{pmatrix} \right\| \leq \phi_n,
\]

and

\[
\left\| \beta^{\text{or}} - \beta^0 \right\| \leq \sqrt{|G_{\text{max}}|} \phi_n; \sup_i \left\| \beta_i^{\text{or}} - \beta_i^0 \right\| \leq \phi_n,
\]

where

\[
\phi_n = c_1^{-1/2} C_1^{-1} M_1 \sqrt{q + Kp} |G_{\text{min}}|^{-1} \sqrt{\frac{\min_i n_i}{n}} \log n.
\]

Furthermore, for any vector \( a_n \in \mathbb{R}^{q+Kp} \), we have as \( n \to \infty \)

\[
\sigma_n(a_n)^{-1} a_n^T \begin{pmatrix} (\hat{\eta}^{\text{or}} - \eta^0)^T, (\hat{\alpha}^{\text{or}} - \alpha^0)^T \end{pmatrix} \overset{d}{\to} N(0, 1),
\]

(15)

where

\[
\sigma_n(a_n) = \sigma \left[ a_n^T (U^T \Omega U)^{-1} U^T \Omega U (U^T \Omega U)^{-1} a_n \right]^{1/2}.
\]

(16)

**Remark 3.** We don't have any specific assumptions about \( n_i \). If \( \min n_i \ll \frac{n}{q+Kp} \log n \), or \( \min n_i = O \left( \frac{n}{q+Kp} \log n \right) \), we have \( |G_{\text{min}}| \gg (q + Kp)^{1/2} \sqrt{\frac{n}{\min_i n_i}} \log n \). If \( \min n_i \gg \frac{n}{q+Kp} \log n \), we have \( |G_{\text{min}}| \gg q + Kp \). In this case, if \( q, p \) and \( K \) are fixed values, what we need is only \( 1/|G_{\text{min}}| = o(1) \).
Remark 4. The model considered in Ma et al. (2018) is a special case of our model, and their condition is a special case of our condition, that is when \( n_i = 1 \).

Remark 5. If let \( |G_{\min}| = \delta n/K \) for some constant \( 0 < \delta \leq 1 \), then
\[
\phi_n = c_1^{-1/2} C_1^{-1} M_1 \delta^{-1} K \sqrt{q + Kp} \sqrt{\log n/(n \min n_i)}.
\]
Moreover, if \( q, p \) and \( K \) are fixed values, then \( \phi_n = C^* \sqrt{\log n/(n \min n_i)} \) for some constant \( 0 < C^* < \infty \).

Next, we study the properties of our proposed estimator. Let
\[
b_n = \min_{i \in G_k, j \in G_{k'}} \| \beta_0^i - \beta_0^j \| = \min_{k \neq k'} \| \alpha_k^0 - \alpha_{k'}^0 \| (17)
\]
be the minimal difference among different groups.

Theorem 2. Suppose the conditions of Theorem 1 hold and \( (C4) \) holds. If \( b_n > a \lambda \) and \( \lambda \gg \phi_n \) for some constant \( a > 0 \), then there exists a local minimizer \( \left( \hat{\eta}(\lambda, \psi)^T, \hat{\beta}(\lambda, \psi)^T \right)^T \) of the objective function \( Q_n(\eta, \beta) \) given in (2) such that
\[
P \left( \left( \hat{\eta}(\lambda, \psi)^T, \hat{\beta}(\lambda, \psi)^T \right)^T = \left( (\eta^0)^T, (\beta^0)^T \right)^T \right) \to 1. \tag{18}
\]

Remark 6. Theorem 2 implies that true group structure can be recovered with probability approaching 1. It also implies that the estimated number of groups \( \hat{K} \) satisfies \( P \left( \hat{K}(\lambda, \psi) = K \right) \to 1 \).

Let \( \hat{\alpha}(\lambda, \psi) \) be the distinct group vectors of \( \hat{\beta}(\lambda, \psi) \). According to Theorem 1 and Theorem 2, we have the following result.

Corollary 1. Suppose the conditions in Theorem 2 hold, for any vector \( a_n \in \mathbb{R}^{q+Kp} \), we have as \( n \to \infty \)
\[
\sigma_n(a_n)^{-1} a_n^T \left( \left( \hat{\eta}(\lambda, \psi) - \eta^0 \right)^T, \left( \hat{\alpha}(\lambda, \psi) - \alpha^0 \right)^T \right)^T \overset{d}{\to} N(0,1). \tag{19}
\]

Remark 7. The variance parameter \( \sigma^2 \) can be estimated by
\[
\sigma^2 = \frac{1}{m - q - Kp} \sum_{i=1}^{n} \sum_{h=1}^{n_i} \left( y_{ih} - z_{ih}^T \hat{\eta} - x_{ih}^T \hat{\beta} \right)^2 \tag{20}
\]

The algorithm can be implemented through package \textit{Spgr} in \url{https://github.com/wangx23/Spgr}. 

10
4 Simulation studies

In this section, we evaluate and compare performance of the proposed SaSa estimator with different weight choices: equal weights $c_{ij} = 1$ (denoted as “equal”), weights defined in (4) (denoted as “reg-sp”), weights defined in (5) (denoted by “reg”), and weights defined in (6) (denoted by “sp”).

The simulations are carried as follows. Let $z_{ih} = (z_{ih,1}, \ldots, z_{ih,5})^T$ with $z_{ih,1} = 1$ and $(z_{ih,2}, \ldots, z_{ih,5})^T$ are generated a multivariate normal distribution with mean 0, variance 1, and pairwise correlation $\rho = 0.3$. Define $x_{ih} = (x_{ih,1}, x_{ih,2})^T$, where $x_{ih,1}$ is simulated from a standard normal distribution and $x_{ih,2}$ is simulated from a centered and standardized binomial $(n, 0.7)$. Let $\eta = (\eta_1, \ldots, \eta_5)^T$, where $\eta_k$’s are simulated from Uniform $[1, 2]$ and standard deviation of the error term is $\sigma = 0.5$. We set $\vartheta = 1$ and $\gamma = 3$ and use the SCAD penalty function. The tuning parameters are chosen by the modified BIC defined by (12). We consider the simulations in several scenarios. The results are based on 100 simulations.

To evaluate subgrouping performance of the proposed method, we report the estimated group number $\hat{K}$, adjusted Rand index (ARI) (Rand, 1971; Hubert and Arabie, 1985; Vinh et al., 2010), and the root mean square error (RMSE) for estimating $\beta$. For the estimated $\hat{K}$ over 100 simulations, we report its average (denoted by “mean”), standard error in the parenthesis, and the occurrence percentage of $\hat{K} = K$ (denoted by “per”). The quantity ARI is used to measure the degree of agreement between two partitions, taking a value between 0 and 1: the larger ARI value, the more agreement. We report the average ARI across 100 simulations along with the standard error in the parentheses. To evaluate estimation accuracy of $\beta$, we also report the average RMSE

$$\sqrt{\frac{1}{n} \sum_{i=1}^{n} \| \hat{\beta}_i - \beta_i \|^2.} \quad (21)$$

4.1 Balanced group

We assume that there are $K = 3$ true groups $\mathcal{G}_1, \mathcal{G}_2$ and $\mathcal{G}_3$. Consider the two spatial settings, for which the group parameters are respectively given by:

Setting 1: $\beta_i = (1, 1)^T$ if $i \in \mathcal{G}_1$; $\beta_i = (1.5, 1.5)^T$ if $i \in \mathcal{G}_2$; $\beta_i = (2, 2)^T$ if $i \in \mathcal{G}_3$.

Setting 2: $\beta_i = (1, 1)^T$ if $i \in \mathcal{G}_1$; $\beta_i = (1.25, 1.25)^T$ if $i \in \mathcal{G}_2$; $\beta_i = (1.5, 1.5)^T$ if $i \in \mathcal{G}_3$.

Under each setting, we simulate the data on two sizes of regular lattice, a $7 \times 7$ grid (left) and a $10 \times 10$ grid (right), as shown in Figure 1. Furthermore, for the $7 \times 7$ grid with $n_i = 10$, we use a 10-fold cross validation to select the tuning parameters. The repeated measures of location $i$ are divided into 10 parts; the $j$th part of each location is combined as the validation data set, the remaining observations form the training data set. The spatial weights (6) are considered. The results are labeled as “cv” in all the tables. Note that “reg_sp” and “reg” were not computed for the $10 \times 10$ grid.
Results for Setting 1: Tables 1, 2 and 3 show the estimated number of groups and ARI. Figures 2 and 3 plot the RMSE of the estimates obtained using different weight choices. After estimating the group structure, one can also estimate parameters $\eta$ and $\beta$ again by assuming that the group information is known; the results are denoted as “refit”. Based on the numerical results, we make the following observations.

First, we summarize the results for the $7 \times 7$ grid. In all the considered scenarios, the spatially weighted penalty outperforms the non-weighed penalty ( “equal”). The upper panels in Tables 1 and 2, the left plot in Figure 2 suggest that, if the number of repeated measurements is relatively small (say, $n_i = 10$), the weights “reg_sp” and “sp” perform similarly and they are the best in terms of estimating $K$, recovering the true subgroup structure (large ARI), and estimating regression coefficients (small RMSE); the weights “equal” and “reg” are much worse. The lower panels of Tables 1 and 2 and the right plot in Figure 2 show that, when the number of repeated measurements gets larger (say, $n_i = 30$), all the methods improve and there is not much difference among them. Cross validation works well in terms of ARI and RMSE, but it tends to overestimate the number of groups $K$. This is because that cross validation focuses more on the prediction accuracy; the coefficient estimates of some groups are close to the true coefficients, but they are not shrank together. In addition, refitting the model does not appear to further improve the accuracy of estimating $\beta$.

Table 1: Summary of the estimate $\hat{K}$ for Setting 1 under the $7 \times 7$ grid.

|      | equal | reg_sp | reg  | sp   | cv   |
|------|-------|--------|------|------|------|
|      | 3.34(0.054) | 3.15(0.039) | 3.33(0.051) | 3.13(0.034) | 3.82(0.13) |
|      | 0.69  | 0.86   | 0.69 | 0.87 | 0.56 |

|      | mean | per  | mean | per  | mean | per  |
|------|------|------|------|------|------|------|
|      | 3.00(0) | 3.00(0) | 3.00(0) | 3.00(0) | 3.00(0) | 3.00(0) |
|      | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
Table 2: Average ARI for Setting 1 under the 7 × 7 grid

|          | equal | reg_sp | reg | sp | cv |
|----------|-------|--------|-----|----|----|
| $n_i = 10$ | 0.80(0.011) | 0.92(0.008) | 0.82(0.01) | 0.92(0.007) | 0.95(0.007) |
| $n_i = 30$ | 0.998(0.001) | 0.999(0.0006) | 0.998(0.001) | 0.999(0.0006) |        |

Figure 2: RMSE for Setting 1 under the 7 × 7 grid

Next, we summarize the results for the 10 × 10 grid. In this case, we consider equal weights and spatial weights only. Again, the spatially-weighted penalty outperforms the non-weighted penalty (“equal”). Table 3 and Figure 3 suggest that, if the number of repeated measurements is relatively small (say, $n_i = 10$), “sp” performs much better in terms of grouping and estimating regression coefficients than “equal”; for a larger number of repeated measurements (say, $n_i = 30$), they perform similarly.

Table 3: Summary of $\hat{K}$ and average ARI for Setting 1 under the 10 × 10 grid.

|          | $\hat{K}$ | ARI |
|----------|------------|-----|
|          | equal | sp | equal | sp |
| $n_i = 10$ | mean | per | 3.59(0.073) | 3.37(0.065) | 0.70(0.009) | 0.97(0.003) |
|          | mean | per | 0.53 | 0.71 | - | - |
| $n_i = 30$ | mean | per | 3(0) | 3(0) | 0.996(0.001) | 1.00(0) |
|          | mean | per | 1.00 | 1.00 | - | - |
Results for Setting 2: In this setting, the group difference becomes smaller. Tables 4, 5 and Figure 4 summarize the results for the $7 \times 7$ grid. For both values of $n_i$, the weights “sp” performs best in terms of estimating the number of groups ($\hat{K}$), recovering the true group structure (ARI), and estimating regression coefficients. In contrast to Setting 1, when the difference among groups becomes smaller, even with $n_i = 30$, the model with the spatial weight is superior to other models.

Table 4: Summary of $\hat{K}$ for Setting 2 under the $7 \times 7$ grid

|        | equal | reg_sp | reg | sp  |
|--------|-------|--------|-----|-----|
| $n_i = 10$ | mean  | 3.25(0.119) | 3.01(0.093) | 3.14(0.107) | 2.88(0.067) |
|        | per   | 0.34   | 0.45 | 0.33 | 0.60  |
| $n_i = 30$ | mean  | 2.70(0.046) | 2.90(0.030) | 2.76(0.043) | 2.95(0.022) |
|        | per   | 0.70   | 0.90 | 0.76 | 0.95  |

Table 5: Average ARI for Setting 2 under the $7 \times 7$ grid

|        | equal | reg_sp | reg | sp  |
|--------|-------|--------|-----|-----|
| $n_i = 10$ | 0.32(0.011) | 0.50(0.023) | 0.33(0.01) | 0.61(0.026) |
| $n_i = 30$ | 0.72(0.018) | 0.86(0.015) | 0.75(0.017) | 0.90(0.012) |
Table 6 and Figure 5 show the results for the 10 × 10 grid. Again, we only compare “equal” weights and “sp” weights. The results suggest similar conclusions to those for the 7 × 7 grid: the model with the spatial weight is superior even with a large number of repeated measurements \( (n_i = 30) \) by producing larger ARI and smaller RMSE.

Table 6: Summary of \( \hat{K} \) and average ARI for Setting 2 under the 10 × 10 grid

\[
\begin{array}{cccccc}
\hline
& \multicolumn{2}{c}{\hat{K}} & \multicolumn{2}{c}{\text{ARI}} \\
& \text{equal} & \text{sp} & \text{equal} & \text{sp} \\
\hline
n_i = 10 & \text{mean} & 3.82(0.146) & 3.35(0.078) & 0.32(0.009) & 0.81(0.022) \\
& \text{per} & 0.32 & 0.620 & - & - \\
\hline
n_i = 30 & \text{mean} & 3.10(0.060) & 3.00(0.0) & 0.79(0.012) & 0.94(0.005) \\
& \text{per} & 0.64 & 1.0 & - & - \\
\hline
\end{array}
\]
4.2 Unbalanced group setting

Here we consider an unbalanced group setting as shown in Figure 6. In this setting, there are four groups, denoted as $G_1, G_2, G_3$ and $G_4$, and two groups have 9 subjects and the other two groups have 41 subjects. The group parameters are $\beta_i = (1, 1)^T$ if $i \in G_1$, $\beta_i = (1.5, 1.5)^T$ if $i \in G_2$, $\beta_i = (2, 2)^T$ if $i \in G_3$ and $\beta_i = (2.5, 2.5)^T$ if $i \in G_4$.

Table 7 and Figure 7 show the summaries of $\hat{K}$, ARI and RMSE for $\beta$ when the number of repeated measurements is $n_i = 10$. Overall speaking, “reg_sp” and “sp” perform better than the other two types of weights. Especially, “sp” performs a slightly better than “reg_sp”. The results are consistent with those under balanced cases. We
expect that, when the group difference becomes smaller, “sp” would still perform better than other weights even when the number of repeated measurements is large.

Table 7: Summary of $\hat{K}$ and average ARI for the unbalanced setting with $n_i = 10$

|       | equal | reg-sp | reg | sp  |
|-------|-------|--------|-----|-----|
| $\hat{K}$ mean | 4.58(0.093) | 4.23(0.049) | 5.17(0.011) | 4.35(0.059) |
| per   | 0.570  | 0.800  | 0.300 | 0.710 |
| ARI mean | 0.62(0.010) | 0.94(0.061) | 0.67(0.009) | 0.96(0.004) |

Figure 7: RMSE for unbalanced setting

4.3 Random group setting

We consider a setting without specified location group information. For each location, it has equal probability to three groups. Table 8 shows the summary of $\hat{K}$ and ARI for Setting 1 under the grid $7 \times 7$ with 10 repeated measures. Table 9 shows the summary of $\hat{K}$ and ARI for Setting 2 under the grid $7 \times 7$ with 30 repeated measures. Figure 8 shows the RMSE results for both cases. We can see that different weights have similar performances. The results suggest that even without prior information on the existence of spatial groups, “sp” weights can still produce comparable results as equal weights.

Table 8: Summary of $\hat{K}$ and average ARI for Setting 1 under the $7 \times 7$ grid with $n_i = 10$

|       | equal | reg_sp | reg | sp  |
|-------|-------|--------|-----|-----|
| $\hat{K}$ mean | 3.42(0.064) | 3.45(0.063) | 3.40(0.059) | 3.45(0.063) |
| per   | 0.66   | 0.62   | 0.65 | 0.62 |
| ARI mean | 0.78(0.011) | 0.82(0.010) | 0.81(0.010) | 0.82(0.011) |
Table 9: Summary of $\hat{K}$ and average ARI for Setting 2 under the $7 \times 7$ grid with $n_i = 30$

|      | equal | reg_sp | reg | sp  |
|------|-------|--------|-----|-----|
| $\hat{K}$ mean per | 2.77(0.045) | 2.77(0.045) | 2.83(0.040) | 2.73(0.047) |
| ARI mean | 0.74(0.015) | 0.76(0.016) | 0.77(0.014) | 0.74(0.017) |

Figure 8: RMSE for random groups under the $7 \times 7$ grid

5 Application

In this section, we apply our SaSa method to an example studying the relationship between two land surveys. In the National Resources Inventory survey (NRI) \(^1\), one main goal is to estimate county level estimates of different land covers, such as cropland, pasture land, urban and forest. Since the NRI county level estimates usually have larger values of coefficient of variation, it would be helpful to include some auxiliary information to improve the estimator. One such set of auxiliary covariates is Cropland Data Layer (CDL), which is based on classification of square pixels into several mutually exclusive and exhaustive land cover categories. We now investigate the relationship between the NRI forest proportion and the CDL forest proportion among 48 states. In NRI, forests belonging to federal land, such as national parks, are not included in the forest category. For states with more forest federal land, NRI estimates would be smaller than CDL estimates. Therefore, different states could have different relationship between these two proportions.

The model we consider is,

$$y_{ih} = \beta_{0,i} + \beta_{1,i}x_{ih} + \epsilon_{ih} \quad (22)$$

\(^1\)https://www.nrcs.usda.gov/wps/portal/nrcs/main/national/technical/nra/nri/
where \( y_{ih} \) is the NRI forest proportion of the \( h \)th county in the \( i \)th state, \( x_{ih} \) is the corresponding CDL forest proportion of the \( h \)th county in the \( i \)th state, and \( \beta_{0,i} \) and \( \beta_{1,i} \) are the unknown coefficients. Both \( x \) and \( y \) are standardized. Instead of using the estimated linear regression coefficients as initial values directly, we use five sets of initial values which are simulated from a multivariate normal distribution with estimated coefficients as the mean vector and estimated covariance matrix as the covariance matrix. The models with the smallest modified BIC values are selected for equal weights and spatial weights respectively.

Figure 9 shows the estimated groups based on 2011 NRI data sets. The left figure plots the estimated groups based on equal weights, and the right one is for the estimated groups based on spatial weights in (6). We find that the two different weights give different estimated groups. Tables 10 and 11 are the corresponding estimates of regression coefficients in different groups.

(a) Estimated groups based on equal weights
(b) Estimated groups based on spatial weights

Figure 9: Estimated groups for both equal weights and spatial weights.

### Table 10: Estimated coefficients of different groups for equal weight

| group | 1  | 2  |
|-------|----|----|
| \( \beta_0 \) | -0.029(0.006) | 0.003(0.008) |
| \( \beta_1 \) | 0.885(0.011) | 0.241(0.026) |

### Table 11: Estimated coefficients of different groups for spatial weights

| group | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|-------|---|---|---|---|---|---|---|
| \( \beta_0 \) | -0.041(0.016) | -0.032(0.006) | 0.003(0.007) | 0.023(0.015) | -0.108(0.283) | 0.275(0.038) | 0.376(0.309) |
| \( \beta_1 \) | 1.018(0.028) | 0.867(0.012) | 0.241(0.024) | 0.608(0.033) | 1.148(0.377) | 0.332(0.064) | 0.341(0.384) |

When considering equal weights, \( \lambda \) is the only tuning parameter in the algorithm. By changing the value of \( \lambda \), we can have different number of groups. We consider to change the \( \lambda \) value in the algorithm based on equal weights such that the number of groups is
the same as what we have selected based on the spatial weights, that is 7 groups. Figure 10 shows the group structure with 7 groups based on equal weights. In both Figure 10 and the left figure of Figure 9, “WA”, “OR” and “CA” are not separated from the majority group (the group with the largest group size) when considering equal weights. These three states are in group 4, which are separated from the majority group (group 2) when considering spatial weights, which is more reasonable and intuitive based on the estimates of regression coefficients as shown in Table 11. Besides that, these three states have more national parks than those states in group 2.

![Figure 10: Estimated groups by changing the tuning parameter $\lambda$ with equal weights.](image)

Alternatively, we also implement $K$-means clustering based on the initial estimates to identify similar behaviors among the states. Figure 11 shows the maps based on 2-means clustering and 7-means clustering, respectively. We notice that the 2-cluster map is almost the same as the map based on equal weights. However, the 7-cluster map is not interpretable compared to the result based on spatial weights. This suggests that the proposed procedure can produce more interpretable subgroup structures than $K$-means clustering methods.
6 Discussion

In this article, we consider the problem of spatial clustering and develop a general framework of spatial automatic subgroup analysis (SaSa) for spatial areal data with repeated measures. In spatial data, since locations near each other usually have similar patterns, we propose to take into account spatial information in the pairwise penalty, where closer locations are assigned with larger weights to encourage stronger shrinkage. In the simulation study, we use several examples to investigate and compare performance of the procedure using different weights and have found that spatial information helps to improve the accuracy of grouping, especially when the minimal group difference is small or the number of repeated measures is small. We also establish theoretical properties of the proposed estimator in terms of its consistency in estimating the number of groups.

In the real data example, we have treated states as locations and counties as repeated measures. Alternatively, one can treat counties as individual units, since one state could have counties with two different features. Then, the algorithm will involve a matrix inverse with dimension more than 3000, which will require higher computational burden. A further study is needed to compare these two models for the application.

Appendices

A Proof of Theorem 1

In this section, we prove Theorem 1. When proving the central limit theorem (CLT) we use the technique in Huang et al. (2004).

The oracle estimator is define in (14), which has the following form

\[
\begin{pmatrix}
\hat{\eta}_{or}^\alpha \\
\hat{\alpha}_{or}
\end{pmatrix} = \left(U^T \Omega U\right)^{-1} U^T \Omega y.
\]
Thus, we have
\[
\begin{pmatrix}
\hat{\eta}^0 - \eta^0 \\
\hat{\alpha}^0 - \alpha^0
\end{pmatrix} = \left(U^T \Omega U\right)^{-1} U^T \Omega \epsilon,
\]
where \(\epsilon = (\epsilon_1^T, \ldots, \epsilon_n^T)^T\) with \(\epsilon_i = (\epsilon_i, \ldots, \epsilon_{i,n})^T\). Therefore,
\[
\left\| \begin{pmatrix}
\hat{\eta}^0 - \eta^0 \\
\hat{\alpha}^0 - \alpha^0
\end{pmatrix} \right\| \leq \left\| \left(U^T \Omega U\right)^{-1}\right\|_2 \left\| U^T \Omega \epsilon \right\|,
\]
where \(\| \cdot \|\) is matrix norm, which is defined as, for a matrix \(A\), \(\|A\|_2 = \sup_{\|x\|_2=1} \|Ax\|\).

We know that
\[
P\left(\left\| U^T \Omega \epsilon \right\|_\infty > C \sqrt{\frac{n}{\min n_i} \log n}\right) \leq P\left(\left\| (XW)^T \Omega \epsilon \right\|_\infty > C \sqrt{\frac{n}{\min n_i} \log n}\right) + P\left(\left\| Z^T \Omega \epsilon \right\|_\infty > C \sqrt{\frac{n}{\min n_i} \log n}\right),
\]
where \(C\) is a finite positive constant and \(\| \cdot \|_\infty\) is defined as, for a vector \(x \in \mathbb{R}^m\), \(\|x\|_\infty = \max_{1 \leq i \leq m} x_i\). By condition (C2), we have
\[
\sqrt{\sum_{i=1}^n \sum_{h=1}^{n_i} \frac{x_{ih}^2}{n_i^2} 1 \{i \in G_k\}} \leq M_1 \sqrt{\sum_{i=1}^n \frac{1}{n_i} \{i \in G_k\}} \leq M_1 \sqrt{\sum_{i=1}^n \frac{1}{n_i}} \leq M_1 \sqrt{\frac{n}{\min n_i}}.
\]

Since
\[
\left\| (XW)^T \Omega \epsilon \right\|_\infty = \sup_{k,i} \left\| \sum_{i=1}^n \frac{1}{n_i} \sum_{h=1}^{n_i} x_{ih} \epsilon_{ih} 1 \{i \in G_k\} \right\|^2,
\]
from condition (C3), it follows that
\[
P\left(\left\| (XW)^T \Omega \epsilon \right\|_\infty > C \sqrt{\frac{n}{\min n_i} \log n}\right)
\leq \sum_{k=1}^p \sum_{i=1}^K P\left(\sum_{i=1}^n \frac{1}{n_i} \sum_{j=1}^{n_i} x_{ih,j} \epsilon_{ih} 1 \{i \in G_k\} > C \sqrt{\frac{n}{\min n_i} \log n}\right)
= \sum_{k=1}^p \sum_{i=1}^K P\left(\sum_{i=1}^n \frac{1}{n_i} \sum_{h=1}^{n_i} x_{ih} \epsilon_{ih} 1 \{i \in G_k\} > \sqrt{\sum_{i=1}^n \sum_{h=1}^{n_i} \frac{x_{ih}^2}{n_i^2} 1 \{i \in G_k\}} \sqrt{\frac{n}{\min n_i} \log n}\right)
\leq 2Kp \exp\left(-c_1 \frac{C^2}{M^2} \log n\right) = 2Kpn^{-c_1 C^2/M^2}.
\]
Similarly, \( \left| \sum_{i=1}^{n} \sum_{h=1}^{n_i} \frac{z_{ih,l}}{n_i} \right| \leq M^2 \sum_{i=1}^{n} 1/n_i \leq M^2 \frac{n}{\min n_i} \). Again, by condition (C3), we have

\[
P \left( \left\| Z^T \Omega \epsilon \right\|_\infty > C \sqrt{\frac{n}{\min n_i}} \log n \right) \leq \sum_{l=1}^{q} \left( \sum_{i=1}^{n} \sum_{h=1}^{n_i} \frac{1}{n_i} z_{ih,l} \epsilon_{ih} \right) > C \sqrt{\frac{n}{\min n_i}} \log n \]

\[
\leq \sum_{l=1}^{q} P \left( \left\| \sum_{i=1}^{n} \sum_{h=1}^{n_i} \frac{1}{n_i} z_{ih,l} \epsilon_{ih} \right\| > \sum_{i=1}^{n} \sum_{h=1}^{n_i} \frac{z_{ih,l}^2}{n_i^2} C \sqrt{\log n} \right)
\leq 2q \exp \left( -c_1 \frac{C^2}{M_1^2} \log n \right) = 2qn^{-c_1C^2/M_1^2}.
\]

Thus, (24) can be bounded by

\[
P \left( \left\| U^T \Omega \epsilon \right\|_\infty > C \sqrt{\frac{n}{\min n_i}} \log n \right) \leq 2q \exp \left( -c_1 \frac{C^2}{M_1^2} \log n \right) = 2qn^{-c_1C^2/M_1^2}.
\]

Let \( C = c_1^{-1/2} M_1 \), thus

\[
P \left( \left\| U^T \Omega \epsilon \right\| > C \sqrt{q + Kp} \sqrt{\frac{n}{\min n_i}} \log n \right) \leq 2 (Kp + q) n^{-c_1C^2/M_1^2}.
\]

(25)

Also, according to condition (C2), we have

\[
\left\| (U^T \Omega) \right\|_{2} \leq C^{-1} |G_{\min}|^{-1}.
\]

(26)

Combining (23), (25) and (26), with probability at least \( 1 - 2 (Kp + q) n^{-1} \), we have

\[
\left\| \left( \hat{\eta}^0 - \eta^0 \right) \right\| \leq CC^{-1} \sqrt{q + Kp} |G_{\min}|^{-1} \sqrt{\frac{n}{\min n_i}} \log n.
\]

Let

\[
\phi_n = c_1^{-1/2} C_1^{-1} M_1 \sqrt{q + Kp} |G_{\min}|^{-1} \sqrt{\frac{n}{\min n_i}} \log n.
\]

Furthermore,

\[
\left\| \beta^0 - \beta^0 \right\|^2 \leq \sum_{k=1}^{K} \sum_{i \in \mathcal{V}_k} \left\| \hat{\alpha}_{k}^{or} - \alpha_{k}^{0} \right\|^2 \leq |G_{\max}| \sum_{k=1}^{K} \left\| \hat{\alpha}_{k}^{or} - \alpha_{k}^{0} \right\|^2
\]

\[
= |G_{\max}| \left\| \hat{\alpha}^{or} - \alpha^{0} \right\|^2 \leq |G_{\max}| \phi_n^2,
\]

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and 
\[ \sup_i \left\| \hat{\beta}_i - \beta_0 \right\| = \sup_k \left\| \hat{\alpha}_k - \alpha_0 \right\| \leq \left\| \hat{\alpha}_0 - \alpha_0 \right\| \leq \phi_n. \]

Next, we consider the central limit theorem. Let \( U = (U_1^T, \ldots, U_n^T)^T \) with \( U_i = (U_{i1}, \ldots, U_{in})^T \) for \( i = 1, \ldots, n \). Consider
\[
a_n \left( (\hat{\omega} - \omega)^T, (\hat{\alpha}_0 - \alpha_0)^T \right)^T = \sum_{i=1}^n \left( \sum_{i=1}^n U_i^T \Omega_i U_i \right)^{-1} U_i^T \Omega_i \epsilon_i,
\]
where \( \Omega_i = 1/n_i I_{n_i} \). By the assumption of \( \epsilon_i \) in the model (1), we have
\[ E \left[ a_n \left( (\hat{\omega} - \omega)^T, (\hat{\alpha}_0 - \alpha_0)^T \right)^T \right] = 0. \]
The variance of \( a_n \left( (\hat{\omega} - \omega)^T, (\hat{\alpha}_0 - \alpha_0)^T \right)^T \) can be written as
\[
Var \left\{ a_n \left( (\hat{\omega} - \omega)^T, (\hat{\alpha}_0 - \alpha_0)^T \right)^T \right\}
= \sigma^2 \left[ a_n \left( U^T \Omega U \right)^{-1} U^T \Omega U \left( U^T \Omega U \right)^{-1} a_n \right]
= \sigma^2 \left[ a_n \left( U^T \Omega U \right)^{-1} \sum_{i=1}^n U_i^T \Omega_i U_i \left( U^T \Omega U \right)^{-1} a_n \right].
\]
We use the technique of Huang et al. (2004) in the proof of their Theorem 3. That is, \( a_n \left( (\hat{\omega} - \omega)^T, (\hat{\alpha}_0 - \alpha_0)^T \right)^T \) can be written as \( \sum_{i=1}^n a_i \xi_i \) with
\[ a_i^2 = a_n \left( U_i^T \Omega U \right)^{-1} U_i^T \Omega_i U_i \left( U_i^T \Omega U \right)^{-1} a_n,
\]
where \( \xi_i \)'s are independent with mean zero and variance one. If
\[ \frac{\max_i a_i^2}{\sum_{i=1}^n a_i^2} \to 0,
\]
then \( \sum_{i=1}^n a_i \xi_i / \sqrt{\sum_{i=1}^n a_i^2} \) is asymptotically \( N(0,1) \).

For any \( \lambda = (\lambda_1, \ldots, \lambda_{q+Kp})^T \), we have
\[
\lambda^T U_i^T \Omega_i U_i \lambda = \frac{1}{n_i} \lambda^T U_i^T U_i \lambda = \frac{1}{n_i} \sum_{h=1}^{n_i} \lambda^T U_{ih} U_{ih}^T \lambda
= \frac{1}{n_i} \sum_{h=1}^{n_i} \left( \sum_{l=1}^{q+Kp} U_{ih,l} \lambda_l \right)^2
\leq \frac{1}{n_i} \sum_{h=1}^{n_i} \left( \sum_{l=1}^{q+Kp} U_{ih,l}^2 \right) \left( \sum_{l=1}^{q+Kp} \lambda_l^2 \right)
\leq \frac{M_1^2}{n_i} (q + Kp) \| \lambda \|^2.
\]

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According to Theorem 1, there exists an event $T$.

In this section, we prove Theorem 2. As in Ma et al. (2018) and Ma and Huang (2017), by assumption.

**Proof of Theorem 2**

Consider the following neighborhood of $(\eta^0, \beta^0)$,

$$
\Theta = \left\{ \eta \in \mathbb{R}^q, \beta \in \mathbb{R}^{np} : \|\eta - \eta^0\| \leq \phi_n, \sup_i \|\beta_i - \beta^0_i\| \leq \phi_n \right\}.
$$

According to Theorem 1, there exists an event $E_1$ where $\|\eta - \eta^0\| \leq \phi_n$ and $\sup_i \|\beta_i - \beta^0_i\| \leq \phi_n$ such that $P(E_1) \geq 1 - 2(q + Kp)n^{-1}$.

Recall that the objective function to minimize is given in (2), which has the following form

$$
Q_n(\eta, \beta; \lambda, \psi) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{n_i} \sum_{h=1}^{n_i} \left( y_{ih} - z_{ih}^T \eta - x_{ih}^T \beta_i \right)^2 + \sum_{1 \leq i < j \leq n} p_i (\|\beta_i - \beta_j\|, c_{ij}, \lambda). \tag{28}
$$

Here we show that $\left((\hat{\eta}^{or})^T, (\hat{\beta}^{or})^T\right)^T$ is a strict local minimizer of the above objective function with probability approaching 1 by two steps as in Ma et al. (2018). The first step is to show that in event $E_1$, $Q_n(\eta, \beta^*) > Q_n(\hat{\eta}^{or}, \hat{\beta}^{or})$ for any $(\eta^T, \beta^T)^T \in \Theta$ and $(\eta^T, \beta^T)^T \neq ((\hat{\eta}^{or})^T, (\hat{\beta}^{or})^T)^T$, where $\beta^* = T^{-1}(T^*(\beta))$ and $\beta \in \mathbb{R}^{np}$. The proof of this step is almost the same as the first step in Ma et al. (2018), which is omitted here.

Here we show the second step, that is, there exists an event $E_2$ such that $P(E_2) \geq 1 - 2n^{-1}$. In the event $E_1 \cap E_2$, there is a neighborhood $\Theta_n$ of $\left((\hat{\eta}^{or})^T, (\hat{\beta}^{or})^T\right)^T$, such that $Q_n(\eta, \beta) \geq Q_n(\eta, \beta^*)$ for any $(\eta^T, \beta^T)^T \in \Theta_n \cap \Theta$ for sufficiently large $n$. 

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Let $\Theta_n = \{\beta_i : \sup_i \|\beta_i - \hat{\beta}_i\| \leq t_n\}$, where $t_n$ is a positive sequence with $t_n = o(1)$.

By Taylor’s expansion, for $(\eta^T, \beta^T)^T \in \Theta_n \cap \Theta$, we have

$$Q_n (\eta, \beta) - Q_n (\eta, \beta^*) = \Gamma_1 + \Gamma_2,$$

where

$$\Gamma_1 = -(y - Z\eta - X\beta^m)^T \Omega X (\beta - \beta^*),$$

$$\Gamma_2 = \sum_{i=1}^n \frac{\partial}{\partial \beta_i^m} \left[ \lambda \sum_{l<j} c_{ij} \rho_j \left( \left\| \beta_i^m - \beta_j^m \right\| \right) \left( \beta_i^m - \beta_j^m \right)^T \left( \beta_i - \beta_j^* \right) \right].$$

with $\beta^m = \alpha \beta + (1 - \alpha) \beta^*$ for some constant $\alpha \in (0, 1)$.

We have $\Gamma_2$ as follows,

$$\Gamma_2 = \lambda \sum_{i<j} c_{ij} \rho_j \left( \left\| \beta_i^m - \beta_j^m \right\| \right) \left( \beta_i^m - \beta_j^m \right)^T \left( \beta_i - \beta_j^* \right) \sum_{k=1}^K \min_{l \in \mathcal{G}_k, j \in \mathcal{G}_{k'}} \left\| \beta_i^0 - \beta_j^0 \right\| - 2 \max_i \left\| \beta_i^m - \beta_i^0 \right\| \geq b_n - 2\phi_n > a\lambda.$$

Thus, $\rho_j \left( \left\| \beta_i^m - \beta_j^m \right\| \right) = 0$ by assumption (C1). Therefore,

$$\Gamma_2 = \lambda \sum_{i=1}^K \sum_{l \in \mathcal{G}_k, i < j} c_{ij} \rho_j \left( \left\| \beta_i^m - \beta_j^m \right\| \right) \left\| \beta_i - \beta_j \right\|. \quad (30)$$

Also, for $i, j \in \mathcal{G}_k$, $\sup_i \left\| \beta_i^m - \beta_j^m \right\| \leq 4t_n$, so $\rho_j \left( \left\| \beta_i^m - \beta_j^m \right\| \right) \geq \rho \left( 4t_n \right)$ by assumption (C1). Thus, we have

$$\Gamma_2 \geq \lambda \sum_{k=1}^K \sum_{i,j \in \mathcal{G}_k, i < j} c_{ij} \rho \left( 4t_n \right) \left\| \beta_i - \beta_j \right\|.$$
Let \( Q = \left( Q_1^T, \ldots, Q_n^T \right)^T = \left[ (y - Z\eta - X\beta^m)^T \Omega X \right]^T \) with

\[
Q_i = \frac{1}{n_i} \sum_{h=1}^{n_i} \left( y_{ih} - z_{ih}^T \eta - x_{ih}^T \beta_i^m \right) x_{ih}.
\]

We have,

\[
\Gamma_1 = -(y - Z\eta - X\beta^m)^T \Omega X (\beta - \beta^*),
\]

\[
= -\sum_{k=1}^{K} \sum_{\{i,j \in G_k, i<j\}} \frac{(Q_i - Q_j)^T (\beta_i - \beta_j)}{|G_k|}.
\]

Moreover,

\[
Q_i = \frac{1}{n_i} \sum_{h=1}^{n_i} \left( \epsilon_{ih} + z_{ih}^T \left( \eta^0 - \eta \right) + x_{ih}^T \left( \beta^0_i - \beta_i^m \right) \right) x_{ih},
\]

so

\[
\sup_i \| Q_i \| \leq \sup_i \| x_{ih} \| \left( \| \xi \|_{\infty} + \sup_i \| z_{ih} \| \| \eta^0 - \eta \| + \sup_i \| x_{ih} \| \| \beta^0_i - \beta_i^m \| \right)
\]

\[
\leq C_2 \sqrt{p} (\| \xi \|_{\infty} + C_3 \sqrt{q} \phi_n + C_2 \sqrt{p} \phi_n),
\]

where \( \xi = (\xi_1, \ldots, \xi_n)^T \) with \( \xi_i = \frac{1}{n_i} \sum_{h=1}^{n_i} \epsilon_{ih} \). According to Condition (C3),

\[
P \left( \| \xi \|_{\infty} > \sqrt{2c_1^{-1} \log n} / \min n_i \right) \leq \sum_{i=1}^{n} P \left( |\xi_i| > \sqrt{2c_1^{-1} \log n} / \min n_i \right)
\]

\[
= \sum_{i=1}^{n} P \left( \left| \frac{1}{n_i} \sum_{j=1}^{n_i} \epsilon_{ij} \right| > \sqrt{2c_1^{-1} \log n} / \min n_i \right)
\]

\[
\leq \sum_{i=1}^{n} P \left( \left| \frac{1}{n_i} \sum_{j=1}^{n_i} \epsilon_{ij} \right| > \sqrt{2c_1^{-1} \log n} / n_i \right)
\]

\[
\leq 2 \sum_{i=1}^{n} \exp \left\{ -c_1 2c_1^{-1} \log n \right\} \leq \frac{2}{n}.
\]

Thus, there exists an event \( E_2 \) such that \( P(E_2) \geq 1 - 2n^{-1} \) and

\[
\sup_i \| Q_i \| \leq C_2 \sqrt{p} \left( \sqrt{2c_1^{-1} \log n} / \min n_i + C_3 \sqrt{q} \phi_n + C_2 \sqrt{p} \phi_n \right).
\]
Thus,
\[
\begin{align*}
\left| \sum_{G_k} \right| \frac{(Q_i - Q_j)^T (\beta_i - \beta_j)}{|G_k|} \leq 2 \|Q_i\| \|\beta_i - \beta_j\|
\end{align*}
\]
\[
\leq 2C_2 |G_{\text{min}}|^{-1} \sqrt{\bar{p}} \left( \sqrt{2c_1^{-1}} \sqrt{\log n/ \min_i n_i} + C_3 \sqrt{\phi_n} + C_2 \sqrt{\rho_n} \right) \|\beta_i - \beta_j\|. \tag{32}
\]

Combining (30), (31) and (32), (29) follows that
\[
Q_n(\eta, \beta) - Q_n(\eta, \beta^*)
\]
\[
\geq \sum_{k=1}^K \sum_{i,j \in G_k, i < j} \left\{ \lambda c_{ij} \rho' (4t_n) - 2C_2 |G_{\text{min}}|^{-1} \sqrt{\bar{p}} \left( \sqrt{2c_1^{-1}} \sqrt{\log n/ \min_i n_i} + C_3 \sqrt{\phi_n} + C_2 \sqrt{\rho_n} \right) \right\} \|\beta_i - \beta_j\|.
\]

As \(t_n = o(1), \rho' (4t_n) \to 1\). Since \(|G_{\text{min}}| \gg (q + Kp)^{1/2} \max \left\{ \sqrt{\frac{n}{\min_i n_i}} \log n, (q + Kp)^{1/2} \right\} \),
\( p = o(n) \) and \( q = o(n) \), then \(|G_{\text{min}}|^{-1} p = o(1) \) and \(|G_{\text{min}}|^{-1} \sqrt{\bar{pq}} = o(1) \). Thus,
\( \lambda \gg |G_{\text{min}}|^{-1} \sqrt{\bar{p}} \left( \frac{\log n}{\min_i n_i} \right) \), \( \lambda \gg |G_{\text{min}}|^{-1} \sqrt{\bar{pq}} \phi_n \) and \( \lambda \gg |G_{\text{min}}|^{-1} p \phi_n \). Therefore, \( Q_n(\eta, \beta) - Q_n(\eta, \beta^*) \geq 0 \) for sufficiently large \( n \) by the assumption (C4) that \( c_{ij} \)’s are bounded if \( i \) and \( j \) are in the same group.

Therefore, combining the two steps, we will have that \( Q_n(\eta, \beta) > Q_n(\hat{\eta}^\text{or}, \hat{\beta}^\text{or}) \) for any \( (\eta^T, \beta^T) \in \Theta_n \cap \Theta \) and \( (\eta^T, \beta^T) \neq ((\hat{\eta}^\text{or})^T, (\hat{\beta}^\text{or})^T)^T \). This shows that
\( ((\hat{\eta}^\text{or})^T, (\hat{\beta}^\text{or})^T)^T \) is a strict local minimizer of the objective function (2) on \( E_1 \cap E_2 \) with probability at least \( 1 - 2(K + p + 1)n^{-1} \) for sufficiently large \( n \).

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