Spatially Clustered Regression

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Abstract

Spatial regression or geographically weighted regression models have been widely adopted to capture the effects of auxiliary information on a response variable of interest over a region, while relationships between response and auxiliary variables are expected to exhibit complex spatial patterns in many applications. In this paper, we propose a new approach for spatial regression, called spatially clustered regression, to estimate possibly clustered spatial patterns of the relationships. We combine K-means based clustering formulation and penalty function motivated from a spatial process known as Potts model for motivating similar clustering in neighboring locations. We provide a simple iterative algorithm to fit the proposed method which is scalable for large spatial datasets. We also discuss two potential extensions of the proposed approach, regularized estimation for variable selection, and semiparametric additive modeling. Through simulation studies, the proposed method is demonstrated to show its superior performance to existing methods even under the true structure does not admit spatial clustering. Finally, the proposed method is applied to crime event data in Tokyo and produces interpretable results for spatial patterns. The R code is available at \url{https://github.com/sshonosuke/SCR}

\textbf{Key words}: Geographically weighted regression; K-means algorithm; Penalized likelihood; Potts model; Spatially varying parameters
1 Introduction

Spatial heterogeneity, which is often referred to as the Second Law of Geography (Goodchild 2004), is ubiquitous in spatial science. Geographically weighted regression (GWR; Brunsdon et al. 1998; Fotheringham et al. 2002), which is a representative approach for modeling spatial heterogeneity, has widely been adopted for modeling possibly spatially varying regression coefficients; its applications cover social science (e.g. Hu et al. 2016), epidemiology (e.g. Nakaya et al. 2005) and environmental science (e.g. Zhou et al. 2019).

Despite the success, GWR is known to be numerically unstable and may produce extreme estimates of coefficients (Wheeler and Tiefelsdorf 2005; Cho et al. 2009). To address the drawback, a wide variety of regularized GWR approaches have been developed (e.g. Wheeler 2007, 2009; Bárčena et al. 2014). More recently, Comber et al. (2016) considered local regularization to enhance accuracy and stability. Still, it is less clear how to regularize GWR to improve stability while maintaining its computational efficiency. Bayesian spatially varying coefficient model (Gelfand et al. 2003; Finley 2011) is another popular approach for modeling spatial heterogeneity in regression coefficients. Wheeler and Waller (2009), Wolf et al. (2018), among others have suggested its stability and estimation accuracy. Yet, this approach can be computationally very intensive for large samples, which limits applications of spatial regression techniques to modern large spatial datasets. Therefore, an alternative method that has stable estimation performance as well as computational efficiency under large datasets is strongly required.

In this paper, we propose a new strategy for spatial regression with possibly spatially varying coefficients or non-stationarity. Our fundamental idea is the combinations of regression modeling and clustering, that is, we assume all the geographical locations can be divided into a finite number of groups, and locations in the same groups share the same regression coefficients, that is, possibly smoothed surface of varying regression coefficients are approximated by step functions. Hence, the results would be numerically stable and could be easier to interpret than those of GWR.
To introduce such a clustering nature, we employ indicators showing the group to which the corresponding location belongs, and we estimate the grouping parameters and group-wise regression models simultaneously. For estimating group memberships, it would be reasonable to impose that the geographically neighboring locations are likely to belong to the same groups, thereby we introduce penalty function to encourage such spatially clustered structure motivated from the hidden Potts model (Potts, 1952) that was originally developed for modeling spatially correlated integers. It will be demonstrated that the proposed objective function can be easily optimized by a simple iterative algorithm which is similar to $K$-means clustering. In particular, updating steps in each iteration do not require computationally intensive manipulations, so that the proposed algorithm is much more scalable than GWR. For selecting the number of groups $G$, we employ an information criterion. Moreover, the proposed approach allows substantial extensions to include variable selection or semiparametric additive modeling, which cannot be achieved by existing approaches such as GWR.

Recently, ideas of combining regression modeling and clustering have been considered in the literature. In the context of spatial regression, Li and Sang (2019) adopted a fused lasso approach to shrink regression coefficients in neighboring areas toward 0, which results in spatially clustered regression coefficients. However, the computation cost under large datasets is very large and the performance is not necessarily reasonable possibly because the method does not take account of spatially heterogeneous variances, which will be demonstrated in our numerical studies. On the other hand, in the context of penal data analysis, clustering approaches using grouping indicators like the proposed method have been widely studied (e.g., Bonhomme and Manresa, 2015; Wang et al., 2018; Ito and Sugasawa, 2020), but the existing works did not take account of spatial similarities among the grouping indicators.

This paper is organized as follows. In Section 2, we introduce the proposed methods, estimation algorithms, and discuss some extensions. In Section 4, we evaluate the numerical performance of the proposed methods together with some existing methods through simulation studies. In Section 5, we demonstrate the proposed method through spatial regression modeling of the number of crimes in the Tokyo metropolitan.
tan area. Finally, we give some discussions in Section 6.

2 Spatially Clustered Regression

2.1 Models and estimation algorithm

Let $y_i$ be a response variable and $x_i$ is a vector of covariates in the $i$th location, for $i = 1, \ldots, n$, where $n$ is the number of samples. We suppose we are interested in the conditional distribution $f(y_i|x_i; \theta_i, \psi)$, where $\theta_i$ and $\psi$ are vectors of unknown parameters. Here $\theta_i$ may change over different locations and represent spatial heterogeneity while $\psi$ is assumed constant in all the areas. For example, $f(y_i|x_i; \theta_i, \psi) = \phi(y_i; x_{i1}^t \theta_i + x_{i2}^t \gamma, \sigma^2)$ with $x_i = (x_{i1}, x_{i2})$ and $\psi = (\gamma, \sigma^2)$. We assume that location information $s_i$ (e.g. longitude and latitude) is also available for the $i$th location. In what follows, we assume that there is no static parameter $\psi$ for simplicity, and all the results given above can be easily extended to the case.

Without any structures for $\theta_i$, we cannot identify these parameters since a repeated measurement on the same location is rarely available in practice. Hence, we assume that $n$ locations are divided into $G$ groups, and locations in the same group share the same parameter values of $\theta_i$. For a while, we treat $G$ as a fixed value, but a data-dependent selection of $G$ will be discussed later. We introduce $g_i \in \{1, \ldots, G\}$, an unknown group membership variable for the $i$th location, and let $\theta_i = \theta_{g_i}$. Then, the distinct values of $\theta_i$’s reduce to $\theta_1, \ldots, \theta_G$, where $\theta = (\theta_1^t, \ldots, \theta_G^t)^t$ is the set of unknown parameters. Therefore, the unknown parameters in the model is the structural parameter $\theta$ and the membership parameter $g = (g_1, \ldots, g_n)^t$.

Regarding the membership parameter, it would be reasonable to consider that the membership in neighboring locations are likely to have the same memberships, which means that the fitted conditional distributions are likely to be the same in the neighboring locations. To encourage such a structure, we introduce a penalty function motivated by a spatial process for discrete space known as the Potts model (Potts, 1952). The same penalty function is firstly adopted in Sugasawa (2020) in the context of mixture modeling. The joint probability function of the Potts model
is given by

\[ \pi(g_1, \ldots, g_n | \phi) \propto \exp \left( \phi \sum_{i < j} w_{ij} I(g_i = g_j) \right), \]

where \( w_{ij} = w(s_i, s_j) \in [0, 1] \), \( w(\cdot, \cdot) \) is a weighting function, and \( \phi \) controls strength of spatial correlation. Note that the normalizing constant in the above distribution is not tractable, but we treat \( \phi \) as a fixed tuning parameter rather than an unknown parameter, so that we do not have to deal with the normalizing constant in the following argument. Since the conditional distribution of \( g_i \) given other variables is the same form as one given above, the conditional distribution put more weights on \( w_{ij} I(g_i = g_j) \) as \( \phi \) is larger. Then, we propose the following penalized likelihood:

\[ Q(\theta, g) \equiv n \sum_{i=1}^{g} \log f(y_i | x_i; \theta_{g_i}) + \phi \sum_{i < j} w_{ij} I(g_i = g_j). \quad (1) \]

The above objective function can be regarded as the logarithm of joint distribution function of \( y_1, \ldots, y_n \) and \( g \). We define the estimator of \( \theta \) and \( g \) as the maximizer of the objective function \( Q(\theta, g) \).

For maximizing the objective function \( (1) \), we may employ a simple iterative algorithm that is similar to K-means clustering which iteratively updates the membership variables \( g \) and other parameters, since the maximization of the objective function \( (1) \) given \( g \) is the same as maximizing the log-likelihood function. The detailed algorithm is given as follows:

**Algorithm 1. (Spatially clustered regression)**

1. Set initial values \( \theta(0) \) and \( g(0) \).

2. Update the current parameter values \( \theta(k) \) and \( g(k) \) as follows:
   
   - Update the group-wise parameter \( \theta_g \) separately for \( g = 1, \ldots, G \):
     
     \[ \theta_g^{(k+1)} = \arg \max_{\theta_g} \sum_{i=1}^{n} I(g_i^{(k)} = g) \log f(y_i | x_i; \theta_g). \]
– Update the membership variable:

\[ g_i^{(k+1)} = \arg \max_{g \in \{1, \ldots, G\}} \left\{ \log f(y_i|x_i; \theta_g^{(k+1)}) + \phi \sum_{j=1; j \neq i}^n w_{ij} I(g = g_j^{(k)}) \right\}. \]

3. Repeat the step 2 until convergence.

Note that the updating step for \( \theta_g \) is the same as maximizing the log-likelihood function based only on data which belongs to the \( g \)th group, thereby this step should be easy as long as the regression model \( f(y_i|x_i; \theta_g) \) is not complicated. For example, when \( f(y_i|x_i; \theta_g) \) is a Gaussian linear regression model, the updating process for \( \theta_g \) are obtained in closed forms. On the other hand, for updating \( g_i \), we just need to calculate values of the penalized likelihood function for all \( g \in \{1, \ldots, G\} \), separately for each \( i \), which is not computation intensive as long as \( G \) is moderate. Therefore, each updating step is quite easy to carry out and computationally less intensive. The convergence in the algorithm is monitored by difference from the current values and updated values, and the algorithm should be terminated when the difference is smaller than the user-specified tolerance value \( \varepsilon \), where we used \( \varepsilon = 10^{-6} \) in our numerical studies.

2.2 Fuzzy clustered regression

Although Algorithm 1 produce interpretable results due to its clustering property, the spatially clustered structure could be restrictive in terms of estimation accuracy when the underlying structure cannot be well approximated by region-wise constant functions. To overcome the difficulty, we consider the smoothed version of the proposed method by incorporating the idea of fuzzy clustering, which allows uncertainty of clustering by introducing smoothed weight determined by the likelihood function. Specifically, we consider the following synthetic probability that the \( i \)th location belongs to group \( g \) given the other group membership variables:

\[ \pi_{iy} = \frac{[f(y_i|x_i; \theta_{g}, \psi) \exp\{\phi \sum_{j=1; j \neq i}^n w_{ij} I(g = g_j)\}]^\delta}{\sum_{g' = 1}^G [f(y_i|x_i; \theta_{g'}) \exp\{\phi \sum_{j=1; j \neq i}^n w_{ij} I(g' = g_j)\}]^\delta}. \]
where $\delta$ controls the degree of fuzziness. As $\delta \to \infty$, the maximum probability among $\{\pi_{i1}, \ldots, \pi_{iG}\}$ would converge to 1, so that the resulting estimation algorithm would be similar to Algorithm 1 when $\delta$ is large. For simplicity, we consider the case with $\delta = 1$ in what follows, and the modified algorithm is given as follows.

**Algorithm 2. (Spatially fuzzy clustered regression)**

1. Set initial values $\theta^{(0)}$ and $g^{(0)}$.

2. Compute the following weights for $i = 1, \ldots, n$ and $g = 1, \ldots, G$.

   $\pi^{(k)}_{ig} = \frac{f(y_i|x_i; \theta^{(k)}_g) \exp \left\{ \phi \sum_{j=1; j \neq i}^n w_{ij} I(g = g^{(k)}_j) \right\}}{\sum_{g'=1}^G f(y_i|x_i; \theta^{(k)}_{g'}) \exp \left\{ \phi \sum_{j=1; j \neq i}^n w_{ij} I(g' = g^{(k)}_j) \right\}}.$

3. Update the current parameter values $\theta^{(k)}$ and $g^{(k)}$ as follows:

   - Update the group-wise parameter $\theta_g$ separately for $g = 1, \ldots, G$:

     $\theta^{(k+1)}_g = \arg\max_{\theta_g} \sum_{i=1}^n \pi^{(k)}_{ig} \log f(y_i|x_i; \theta_g).$

   - Update the membership variable: $g^{(k+1)}_i = \arg\max_{g \in \{1, \ldots, G\}} \pi^{(k)}_{ig}$.

4. Repeat the steps 2 and 3 until convergence.

Note that the updating step for $\theta_g$ corresponds to maximizing the weighted objective function, which is easy for typical regression models. The updating processes for $\pi_{ig}$ and $g_i$ can be also easily carried out without any computational difficulty. Based on the outputs from Algorithm 2, we can compute the smoothed estimator of $\theta_i$ as $\hat{\theta}_i = \sum_{g=1}^G \hat{\pi}_{ik} \hat{\theta}_g$. Although this smoothed estimator does not hold a clustering nature due to area-wise mixing rates $\hat{\pi}_{ik}$, it can be more flexibly adapted to local changes of underlying spatially varying parameters.

### 2.3 Selection of tuning parameters

In the proposed method, we have two tuning parameters, $G$, the number of groups, and $\phi$ controlling the strength of spatial dependence of $g_i$s. Since we found that the
specific choice of $\phi$ is not very sensitive as long as $\phi$ is strictly positive, thereby we simply recommend setting $\phi = 1$. Although the number of groups, $G$, could be determined according to the prior information regarding the dataset, a data-dependent method can be employed by using the following information criterion:

$$IC(G) = -2 \sum_{i=1}^{n} \log f(y_i|x_i; \hat{\theta}_{g_i}) + c_n \dim(\theta), \quad (2)$$

where $c_n$ is a constant depending on the sample size $n$ and $\dim(\theta)$ denotes the dimension of $\theta$ which depends on $G$. Specifically, we use $c_n = \log n$ which leads to a BIC-type criterion. We select a suitable value of $G$ as $\hat{G} = \arg\min_{G \in \{G_1, \ldots, G_L\}} IC(G)$, where $G_1, \ldots, G_L$ are candidates of $G$.

3 Extensions

3.1 Variable selection via regularization

The number of regression coefficients in the proposed model is $pG$, where $p$ is the dimension of coefficient vectors in each group. Hence, if $p$ is not small, it would be better to select a suitable subset of the regression coefficients to make the estimation result more interpretable as well as to enhance prediction accuracy. To this end, we can combine regularized estimation techniques such as Lasso [Tibshirani 1996] in the objective function (1), given by

$$\sum_{i=1}^{n} \log f(y_i|x_i; \theta_{g_i}) + \phi \sum_{i<j} w_{ij} I(g_i = g_j) - \lambda \sum_{g=1}^{G} \sum_{k=1}^{p} \text{pen}(\theta_{gk}), \quad (3)$$

where $\lambda$ is a tuning parameter and $\text{pen}(\cdot)$ is a penalty function, e.g. $\text{pen}(x) = |x|$ for Lasso regularization. Under the formulation, the updating step for $\theta$ in Algorithm 1 is changed as follows:

$$\theta^{(k+1)}_g = \arg\max_{\theta_g} \left\{ \sum_{i=1}^{n} I(g_i^{(k)} = g) \log f(y_i|x_i; \theta_g) - \lambda \sum_{k=1}^{p} \text{pen}(\theta_{gk}) \right\}. \quad (3)$$
The above objective function is the same as the penalized log-likelihood based only on the data in the \( g \)th group, thereby efficient computation algorithms are already available for some specific penalty functions.

It should be noted that the use of the objective function (3) leads to different selected variables in each group. Thus (3) does not necessarily induce variable selection of the \( p \) variables in \( x_i \). In practice, it would be more useful to determine the variable which is not used in all the \( G \) models. To this end, we also suggest using a grouped penalty function \( \sum_{k=1}^{p} \text{pen}(\theta_{1k}, \ldots, \theta_{Gk}) \) instead of the element-wise penalty adopted in (3), where \( \text{pen}(\theta_{1k}, \ldots, \theta_{Gk}) \) is the simultaneous penalty on \( G \) regression coefficients of the \( k \)th variable. A standard choice would be grouped lasso penalty\footnote{Yuan and Lin 2006} given by \( \sqrt{\sum_{g=1}^{G} \theta_{gk}^2} \).

In both formulations, there is a tuning parameter \( \lambda \) that should be properly choosen to make reasonable regularized estimation. Following\footnote{Zhou et al. 2007}, we replace \( \dim(\theta) \) with the degrees of freedom \( \sum_{g=1}^{G} \sum_{k=1}^{p} I(\hat{\theta}_{gk} \neq 0) \) in (2). In this case, the information criterion is a function of \( G \) and \( \lambda \), and the minimizer among some candidates of \((G, \lambda)\) should be adopted.

### 3.2 Semiparametric additive modeling

More flexible modeling can be achieved by adopting semiparametric techniques for estimating conditional distributions. Suppose the conditional expectation is expressed as the additive form \( m(E[y_i|x_i]) = \sum_{k=1}^{p} h_{gk}(x_{ik}) \), where \( m(\cdot) \) is some specified link functions. Then, the conditional distribution can be expressed as \( f(y_i|x_i; H_{g}, \gamma_{g}) \), where \( H_{g} = \{ h_{g1}, \ldots, h_{gp} \} \) is a collection of unknown \( p \) functions and \( \gamma \) is a dispersion parameter. For example, the linear additive model is expressed as \( y_i \sim N(\sum_{k=1}^{p} h_{gk}(x_{ik}), \sigma_{g}^2) \), so that \( E[y_i|x_i] = \sum_{k=1}^{p} h_{gk}(x_{ik}) \). In the above model, the additive effect of each covariate can be different among \( G \) groups, and the model can be seen as semiparametric version of the model discussed in Section 2. To estimate the model, we slightly modify Algorithm 1 (Algorithm 2 can also be modified in the same manner). The updating step of \( g_i \) in the \( k \)th step is not changed,
while the updating step for $H_g$ is given by

$$H_g^{(k+1)} = \arg \max_{H_g} \sum_{i=1}^{n} I(g_i^{(k)} = g) \log f(y_i| x_i; H_g, \gamma_g^{(k)}).$$

The above optimization step is nothing but fitting the generalized additive models for observations assigned to the $g$th group, so that standard techniques such as sequential fitting (e.g. Hastie and Tibshirani 1986) can be adopted to obtain $H_g^{(k+1)}$. The dispersion parameter $\gamma$ can be updated in the same manner.

4 Simulation Studies

4.1 Simulation settings

We present simulation studies to illustrate the performance of the proposed spatially clustered regression (SCR) and spatially fuzzy clustered regression (SFCR) methods under two scenarios for underlying structures of regression coefficients. In both scenarios, we uniformly generated 1000 spatial locations $s_1, \ldots, s_n$ in the domain

$$\{ s = (s_1, s_2) \mid s_1 \in [-1, 1], \ s_2 \in [0, 2], \ s_1^2 + 0.5s_2^2 > (0.5)^2 \}.$$  

Then, we generated two covariates from spatial processes, following Li and Sang (2019). Let $z_1(s_i)$ and $z_2(s_i)$ be the two independent realizations of a spatial Gaussian process with mean zero and a covariance matrix defined from an isotropic exponential function:

$$\text{Cov}(z_k(s_i), z_k(s_j)) = \exp(-\|s_i - s_j\|/\eta), \ k = 1, 2,$$

where $\eta$ is the range parameter. We considered three cases of the parameter, $\eta = 0.2, 0.6, 1$, which are referred to as weak, moderate, and strong spatial correlation. Then, we define two covariates $x_1(s_i)$ and $x_2(s_i)$ via linear transformations

$$x_1(s_i) = z_1(s_i) \quad \text{and} \quad x_2(s_i) = rz_1(s_i) + \sqrt{1-r^2}z_2(s_i)$$

with $r = 0.75$, which allows dependence between $x_1(s_i)$ and $x_2(s_i)$. Then, the response at each location is generated from the following model:

$$y(s_i) = \beta_0(s_i) + \beta_1(s_i)x_1(s_i) + \beta_2(s_i)x_2(s_i) + \sigma(s_i)\varepsilon(s_i), \quad i = 1, \ldots, n,$$

where $\varepsilon(s_i)$’s are mutually independent and $\varepsilon(s_i) \sim N(0, 1)$. Regarding the settings of the regression coefficients and error variance, we considered the following two sce-
narios:

- **(Scenario 1: Spatially clustered parameters)** The sampled domain is divided into 6 regions $D_{jk} = \{ s \mid g_{1j} < s \leq g_{1j+1}, \ g_{2k} < s \leq g_{2k+1} \}$ for $j = 0,1$ and $k = 0,1,2$, where $g_{1j} = -1 + j$ and $g_{2k} = 2k/3$. Regression coefficients and error variance for locations in $D_{jk}$ are set as follows:

$$
\begin{align*}
\beta_0(s_i) &= 2(g_{1j} + g_{2k}), \\
\beta_1(s_i) &= g_{1j}^2 + g_{2k}^2, \\
\beta_2(s_i) &= -g_{1j} - g_{2k}, \\
\sigma(s_i) &= 0.5 + 0.2|g_{1j} - g_{2k}|,
\end{align*}
$$

thereby the regression coefficients and error variance are constant within the region $D_{jk}$.

- **(Scenario 2: Spatially smoothed parameters)** Each regression coefficient was independently generated from a Gaussian spatial process. We set that all the processes have a zero mean and isotropic exponential function given by

$$
\text{Cov}(\beta_k(s_i), \beta_k(s_j)) = \tau^2 \exp\left(-\frac{\|s_i - s_j\|}{\psi_k}\right), \quad k = 0,1,2,
$$

where $\psi_k$ is the range parameter and $\tau^2$ is the variance parameter. We fix $\tau^2 = 2$ and $\psi_k = k+1$ in our study. Regarding the error variance, we set $\sigma(s_i) = 0.2 \exp(u(s_i))$, where $u(s_i)$ is a zero mean Gaussian spatial process with the same isotropic exponential function $\text{Cov}(u_k(s_i), u_k(s_j)) = (0.5)^2 \exp(-\|s_i - s_j\|/3)$.

4.2 Methods

For the simulated dataset, we applied the proposed SCR with $w_{ij} = I(\|s_i - s_j\| < 0.1)$, $\phi = 1$ and the number of groups $G$ selected among $\{5,10,\ldots,30\}$ by using the BIC-type criterion [2]. In scenario (II), we also applied SFCR with $\delta = 1$, where the same selected value of $G$ in SCR was adopted. For competitors, we adopted two methods. The first one is geographically weighted regression (GWR) as the most standard method in spatial regression. Although spatially varying coefficient models [Gelfand et al., 2003] are also standard methods, previous studies suggest
that spatially varying coefficient models tend to produce similar results to those of GWR (Finley, 2011) since they can be regarded as a model-based version of GWR. Therefore, we only adopted GWR in this study. The bandwidth parameter in GWR was chosen via cross-validation, and all the estimation procedure was carried out via R package “spgwr” (Bivand and Yu, 2020). The second comparative approach is a more advanced and recent regularization technique called spatially homogeneity pursuit (SHP) proposed in Li and Sang (2019). In this method, we first constructed a minimum spanning tree connecting all the locations using R package “ape” (Paradis and Schliep, 2019), and then lasso regularized estimation is applied using R package ”glmnet” (Friedman et al., 2010). Following Li and Sang (2019), the tuning parameter in the regularized estimation was selected by the BIC-type criterion. The estimation performance is evaluated based on the mean squared error (MSE) given by

\[
\text{MSE} = \frac{1}{np} \sum_{i=1}^{n} \sum_{k=0}^{p-1} \left(\hat{\beta}_k(s_i) - \beta_k(s_i)\right)^2,
\]

where \(p = 3\) and \(\hat{\beta}_k(s_i)\) is the estimated value of \(\beta_k(s_i)\).

4.3 Results

We first show the result in one simulation with \(\phi = 0.2\). In Table 1 we reported the computation time (second) of each method, where the program was run on a PC with a 3 GHz 8-Core Intel Xeon E5 8 Core Processor with approximately 16GB RAM. It is observed that the proposed method is computationally comparable with GWR whereas SHP is computationally much more intensive than the other methods. In the SHP method, we found that computation time for the minimum spanning tree accounts for a large portion of the total computation time of SHP. The spatial patterns of the true and estimated parameter values are presented in Figures 1 and 2.

In scenario 1, the proposed method can successfully capture the underlying clustered structures of the regression coefficients and detects the abrupt changes across the boundaries of adjacent clusters. Note that the selected number of groups was \(G = 10\) which is the smallest choice among candidates that are larger than the true number.
of clusters. On the other hand, GWR does not provide estimates having clustered structure and produces poor estimates in some locations. Although SHP can capture similar clustered structures, the proposed SCR can more precisely capture the structure. In scenario 2, it is observed that GWR can precisely estimate the spatially smoothed regression coefficients while SCR can also produce reasonable estimates by allowing a large number of groups. In fact, the largest number \( G = 30 \) among the candidates is selected in this scenario. Moreover, SFCR produces more smoothed estimates than SCR, which are more similar to ones by GWR. In contrast, the results of SHP are not necessarily satisfactory compared with the other methods.

We next evaluated estimation performance based on 1000 simulated datasets under weak \( (\eta = 0.2) \), moderate \( (\eta = 0.6) \) and strong \( (\eta = 1) \) spatial correlation in covariates. The boxplots of MSE are given in Figure 3. In scenario 1, SCR works better than GWR regardless of the strength of spatial correlation due to the underlying clustered structures of regression coefficients. Although SHP takes account of clustered structures, the performance is not necessarily preferable compared with the other methods possibly because SHP implicitly assumes that the error variance is spatially homogeneous. It is also observed that the performance of GWR under moderate or strong spatial correlation in covariates is not satisfactory. In scenario 2, the proposed methods (SCR and SFCR) and GWR are quite comparable when the spatial correlation in covariates is weak, whereas the proposed methods tend to perform better than GWR as the spatial correlation increases. Although the performance of SHP is not preferable under a weak spatial correlation, the relative performance gets improved as the spatial correlation increases. Comparing SCR (hard clustering version) and SFCR (fuzzy clustering version), SFCR can provide slightly better estimates than SCR since the true spatial patterns are smooth.

In summary, the proposed method can produce spatially varying estimates that are more precise or as precise as those of the existing methods, while the computation time is comparable with GWR and is much smaller than SHP. Hence, the proposed method would be a preferable alternative for flexible spatial regression under a large spatial dataset.
4.4 Computation time under large spatial data

Finally, we evaluated the scalability of the proposed method under large spatial datasets compared with GWR. In this study, we set $\eta = 0$ (no spatial correlations in covariates), scenario 1 for the regression coefficients, and considered five cases of the sample size, namely, $n \in \{1000, 3000, 5000, 10000, 20000\}$. For each $n$, we generated 20 datasets and applied GWR, SCR, and SFCR, where the tuning parameter was selected in the same way as in Section 4.2. The averaged value and actual ranges of computation times over 20 replications are shown in Figure 4. The results clearly reveal that the computation time of GWR rapidly increases as $n$ increases while both SCR and SFCR are rather scalable even under large $n$ situations. In fact, the computation time of GWR under $n = 1000$ is around four times longer than those of SCR and SFCR, but that of GWR under $n = 20000$ is more than 20 times longer than those of SCR and SFCR.

Table 1: Computation time (seconds) of the four methods in one simulation.

| Scenario | GWR | SHP | SCR | SFCR |
|----------|-----|-----|-----|------|
| Scenario 1 | 4.1 | 93.0 | 3.5 | -- |
| Scenario 2 | 4.3 | 87.0 | 1.4 | 2.2 |

5 Application to crime risk modeling

Here we apply the proposed methods to a dataset of the number of police-recorded crime in the Tokyo metropolitan area, provided by the University of Tsukuba and publicly available online ("GIS database of the number of police-recorded crime at O-aza, chome in Tokyo, 2009-2017", available at [https://commons.sk.tsukuba.ac.jp/data_en](https://commons.sk.tsukuba.ac.jp/data_en)). In this study, we focus on the number of violent crimes in $n = 2,855$ local towns in the Tokyo metropolitan area in 2015. For auxiliary information about each town, we adopted area (km$^2$), entire population density (PD), day-time population density (DPD), the density of foreign people (FD), percentage of single-person household (SH), and average year of living (AYL). Let $y_i$ be the observed
count of violent crimes, $a_i$ be area and $x_i$ be the vector of standardized auxiliary information in the $i$th local town. We are interested in factor analysis of the number of crimes based on these covariates. To this end, we employed the following spatially clustered Poisson regression model:

$$y_i \sim \text{Po}(a_i \lambda_i), \quad \lambda_i = \exp(x_i^T \beta_{g_i}),$$

(4)
Figure 2: Scenario 2: spatial patterns of true and estimated regression coefficients based on GWR, SHP, SCR, SFCR in one simulation with the spatial range parameter $\eta = 0.2$ for covariates.
We can also access to geographical locations of each area, that is, longitude and latitude of center locations, denoted by $s_i$. Based on the information, we regarded $i$th and $j$th locations are neighbor if $\|s_i - s_j\|$ is smaller than 0.15, which leads to contingency matrix. The average number of neighboring areas was 7.8.

We applied the SCR method with Lasso regularization presented in Section 3.1. We set $\phi = 1$ and selected combinations of $G$ and $\lambda$ from $G \in \{15, \ldots, 30\}$ and $\lambda \in \{0, 0.01, 0.02, \ldots, 0.1\}$ based on the BIC-type criterion [2]. Then, we obtained $G = 18$ and $\lambda = 0.09$ as the optimal choice. Using the tuning parameters, we applied the proposed SCR as well as SFCR to the dataset. For comparisons, we also applied GWR with Poisson regression with two choices of bandwidth, 0.2, and 0.3, denoted by GWR1 and GWR2, respectively. In Figure 5, we reported the estimated spatially regression coefficients for all the covariates. It is observed that GWR1 produces estimates that change drastically over the space, and the change tends to be more drastic around the edge of the space, which would be because there is no sufficient informa-
tion to stably estimate the regression coefficients with a bandwidth of $h = 0.2$. The use of a larger value of bandwidth (GWR2) seems to provide slightly over-smoothed estimates of DPD and PFD while the change of estimates around the edge is still slightly drastic. On the other hand, the proposed SCR method provides reasonable spatial clustering results as well as estimates of group-wise regression coefficients. Specifically, it is observed that SCR can produce exactly 0 estimates of the regression coefficients owing to the Lasso regularization, which cannot be directly imported into GWR frameworks. For example, it can be seen that DPD does not have an effect on the crime rate in the west and east regions, which makes the interpretation of the result much easier. It is also noted that the estimates of SCR, GWR1, and GWR2 are relatively similar in the central part where the parameters are expected to be stably estimated by GWR, which would indicate that SCR provides reasonable estimates. Finally, SFCR provides slightly more smoothed estimates than SCR especially

Figure 4: Computation time (seconds) of GWR, SCR and SFCR under large samples, which are averaged over 20 replications. The vertical lines represent actual ranges of computation times of 20 replications.
around the boundaries between clusters and the estimates cannot be exactly 0 due to the averaging nature of SFCR, but estimates by SFCR are still very close to 0 in locations where the estimates by SCR are exactly 0.

Figure 5: Estimates of spatially varying coefficients for the five covariates, PD, DPD, FD, SH, and AYL based on geographically weighted regression (GWR), spatially clustered regression (SCR), and spatially fuzzy clustered regression (SFCR). Coefficients with exactly 0 estimates are shown by grey.
6 Concluding remarks

This paper proposes a new spatial regression technique, called spatially clustered regression (SCR), with accounting for spatial heterogeneity in model parameters by explicitly introducing grouping parameters. By employing a penalty function motivated from the Potts model, we formulated the penalized likelihood function that can be easily maximized via a simple iterative algorithm. We also developed a fuzzy version of the method that can produce more spatially smoothed estimates, and considered straightforward but important extensions of the main idea. Compared with the most standard technique, GWR, we numerically confirmed that SCR performs better than or as well as GWR in terms of parameter estimation, and the computational cost of SCR is much smaller than that of GWR under large spatial data.

As a potential limitation of SCR, there seems no reasonable way to obtain a measure of uncertainty quantification (e.g. standard errors or confidence intervals) for the model parameters as well as the grouping parameters. One simple approach is to split the data by the estimated grouping parameters and then apply the standard likelihood-based inference techniques to each group-specific parameter. However, this method ignores the uncertainty of grouping. Although it might be useful to employ bootstrap techniques to make statistical inferences on all the parameters including grouping, the detailed procedure for bootstrap in this context is not necessarily clear. We left these issues as interesting future studies.

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