A generalized regionalization framework for geographical modelling and its application in spatial regression

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ABSTRACT
Models applied to geographic data face a trade-off between producing general results and capturing local variations due to spatial heterogeneity. Spatial modelling within carefully defined regions offers an intermediate position between global and local models. However, current spatial optimization approaches to delineate homogeneous regions consider the similarity of attribute values, thus unable to identify regions with similar data generation processes described by geographical models. We propose a generalized regionalization framework, which optimizes region delineation corresponding to a model with region-specific parameters. Within this framework, we introduce three regionalization algorithms, namely automatic zoning procedure (AZP), K-Models, and Regional-K-Models. We adopt an objective function that jointly minimizes modelling errors and the complexity of the region scheme. Results from regression experiments indicate that the K-Models algorithm reconstructs the regions better than the baseline, according to Rand index and mutual information measures. Our suggested framework contributes to better capturing processes exhibiting spatial heterogeneity and may be applied to a wide range of modelling scenarios.

KEYWORDS
Regionalization; spatial heterogeneity; geographical modelling; spatial regression

1. Introduction

Along with spatial dependency, spatial heterogeneity is one of the two fundamental properties of spatial data, commonly observed in both natural and social phenomena [Anselin 1988, Shaver 2005, Fotheringham and Sachdeva 2022]. Spatial heterogeneity can be observed in varying attribute values across space, and in the geographic processes that generate the attribute data. In other words, principles and laws in social and environmental sciences usually do not hold across large spatial domains and scales, in contrast to physics or chemistry. Replicability, which is the ability to obtain consistent results using similar data and methods, is therefore difficult to reach strictly in geographic studies [Goodchild and Li 2021, Sui and Kedron 2021]. Yet replicability may be partially achieved by allowing some aspects of a geographical model (e.g.
its estimated parameters) to vary across space, while keeping its structure (e.g. the set of features) replicable. This partial replicability refers to the concept of “weak replicability” (Goodchild and Li 2021, Liu et al. 2022).

A global model fitted for a whole study area may estimate an overall trend across space, unable to capture regional heterogeneity. As a result, the modelling accuracy (measured by errors between observed data and model output) may be unsatisfying. In contrast, local models may explicitly account for spatial heterogeneity by allowing model parameters to vary across space. A well-known example is geographically weighted regression (GWR, Brunsdon et al. (1996)) and its extension, multiscale GWR (Fotheringham et al. 2017). In line with the concept of weak replicability (Goodchild and Li 2021), the model specification of GWR does not change in a study area, while its parameters are allowed to vary across different locations. Yet the flexibility gained by introducing local parameters ineluctably affects the ability of local models to capture general patterns. Moreover, the pointwise model representation is not parsimonious, with much more total parameters than a global model.

Regional models offer an intermediate approach positioned between global and local modelling. In this framework, the study area is divided into a set of zones, which are usually required to be spatially contiguous, and a set of model parameters is calibrated for each zone. The spatial contiguity constraint reflects the principle of spatial dependency formulated in Tobler’s first law of geography (Tobler 1970). Since near locations tend to exhibit similar geographical properties and processes, aggregating neighboring spatial units into regions may find a compromise between the accuracy and parsimony of the model.

Nevertheless, the task of delineating regions is not trivial. Duque et al. (2011) formalize the regionalization task as the $p$-regions problem, which aims to aggregate a set of spatial units into a set of spatially contiguous regions, following optimization criteria. The mixed integer programming (MIP) approach may solve this problem exactly, yet it is computationally expensive and therefore only applicable to small datasets (e.g., 5×5 grids) (Duque et al. 2011). Heuristic methods have been developed as a computationally-efficient alternative to exact procedures, such as the automatic zoning procedure (AZP) (Openshaw 1977, Openshaw and Rao 1995), spatial ‘$k$’-cluster analysis by tree edge removal (SKATER) (Assunção et al. 2006), and regionalization with dynamically constrained agglomerative clustering and partitioning (REDCAP) (Guo 2008).

However, current spatial optimization approaches have mostly focused on attribute-based regionalization, which aggregates spatial units with similar observed features into a region. These methods do not consider the underlying processes that generated the data, and therefore, are unable to capture and quantify the role of potential drivers that may jointly lead, along with spatial dependency, to spatial clusters. These limitations are especially problematic in environmental and social studies, where the mechanisms leading to spatial clusters are often the result of complex factors. Examples include temperature-salinity relationship of seawater (Luo et al. 2021), and the effect of precipitation on plague intensity (Xu et al. 2011), which require identifying regions with homogeneous geographic processes rather than attribute values.

Model-based clustering methods aim to detect clusters in latent regression coefficients, which represents a homogeneous area with respect to relationship between variables. These include Dirichlet processes models (Ma et al. 2020), Bayesian parti-

\footnote{Here a regional model refers to a model which is applied in a region (a geographically connected part of the study area). Throughout this paper, we assume model specification is fixed, while the model parameters are allowed to vary across regions.}
tion models based on Voronoi tessellation (Zhang et al. 2014), and spatially clustered coefficients regression (Li and Sang 2019). Yet these methods cannot consider regions with arbitrary shapes, or tend to produce many small areas, thus are not qualified as regionalization algorithms (Luo et al. 2021). Recently developed Bayesian spatially clustered coefficient model (BSCC) overcame these issues (Luo et al. 2021). However, the determination of the priors on all parameters may be challenging for non-experts or without a priori knowledge. Furthermore, the fitting process is computationally demanding and would require alternatives to MCMC approaches to accommodate large datasets.

We propose a generalized regionalization framework which can account for the geographical processes that generate the data and the associated regions, where attribute-based regionalization is a special case. Our framework can accommodate a large variety of geographic models, such as spatial linear regression, gravity models for spatial interaction data, or pixel-based classifier for remote sensing imagery. We introduce a two-item objective function which accounts for the trade-off between model accuracy and parsimony. If two regionalization schemes result in similar overall accuracy, the scheme with less regions is preferred. Our approach represents an extension to current spatial optimization approaches for regionalization, and a potentially faster and more scalable alternative to state-of-the-art model-based regionalization methods such as BSCC.

We compared the performance of three regionalization algorithms in their ability to optimize the objective function and reconstruct regions. We consider one existing algorithm (AZP) and two extended algorithms based on K-Means and Regional-K-Means (Feng et al. 2021), which we entitled K-Models and Regional-K-Models. AZP does not require particular extension, while K-Means and Regional-K-Means algorithms are extended as they are only applicable to attribute-based regionalization. We conducted experiments on both simulated and real datasets within a linear regression context, where the spatial units are aggregated based on processes that generate the data, specified in linear regression models, instead of the attribute values.

2. Related works

Regionalization can be viewed as a specific spatial clustering procedure aiming at aggregating spatial units into geographically connected regions (Wei et al. 2022). After the regionalization procedure, each unit is assigned to a unique region, and each region contains at least one unit (Duque et al. 2007). The number of regions is often predefined, although some framework such as max-p-regions (Duque et al. 2012) treats it as an endogenous variable. The criteria used to identify the regions may include equity or threshold of attributes (Duque et al. 2012), compactness of geometry (Li et al. 2014), spatial auto-correlation (Openshaw and Rao 1995), or goodness-of-fit of a global model (Openshaw 1978). Note that our regional modelling approach differs from Openshaw (1978), where a global model is fitted and each region is treated as an individual data point.

A basic criterion for regionalization is homogeneity, which assumes that spatial units in a region are similar, while those in different regions are distinct. This is in line with generic clustering analysis in unsupervised machine learning. We consider two types of regionalization based on homogeneity: attribute-based and model-based regionaliza-

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2For example, the population in each region is required be as similar as possible or above a predefined value. See Duque et al. (2012), Folch and Spielman (2014), Wei et al. (2021).
tion. Attribute-based approaches delineate regions with homogeneous attribute values, which is the usual case of regionalization. Model-based approaches consider homogeneity of the underlying spatial process that generates the data, which is represented by robustness in the parameter estimation of a model across a region. For example, consider a simple linear regression model expressed as $y_i = \beta i x_i + \epsilon_i$, $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$, with a dependent variable $y_i$ and an independent variable $x_i$ associated with a linear coefficient $\beta_i$ allowed to vary for each spatial unit $u_i$ within a region $R_j$ in a spatial domain $\mathcal{D}$. The region $R_j$ is considered homogeneous if the estimated parameters are similar for each spatial unit within $R_j$ ($\beta_i \approx \beta$, $\forall u_i \in R_j$), which indicates similar relationship between $y_i$ and $x_i$ across the region. We suppose that attribute-based and model-based regionalization could be formalized in a unified manner, and solved with the same generalized zone design algorithms, as in the proposed framework.

For attribute-based regionalization, assume $y_i$ is the attribute vector associated with spatial unit $u_i$ ($i = 1, 2, \ldots, N$). Current methods usually minimize an objective function of the sum of within-region variability across all delineated regions (Equation 1):

$$L(R) = \sum_{j=1}^{M} \sum_{1 \leq i_1 < i_2 \leq N} I[u_{i_1}, u_{i_2} \in R_j] \|y_{i_1} - y_{i_2}\|_2,$$

(1)

where $R = \{R_j\}_{j=1}^{M}$ is the set of regions in a spatial domain $\mathcal{D}$; $I[\text{cond}]$ is an indicator function, which takes 1 if the condition (cond) is true, 0 otherwise; $\| \cdot \|$ represents a vector norm, commonly formulated as Euclidean $L_2$-norm. Based on how spatial contiguity is treated, existing algorithms may be classified into two main categories, spatially implicit methods and spatially explicit methods (Duque et al. 2007).

Spatially implicit methods first apply a generic clustering algorithm to the set of attribute vectors, without necessarily defining geographically connected regions. Post-processing steps are performed afterwards to impose spatial contiguity on each region. To achieve spatial contiguity, non-connected regions may be broken into connected parts (Openshaw and Wymer 1995). After that, manual refinement may be performed. Spatially implicit methods are less preferred in some occasions, as they do not allow a strict control of the number of regions (post-processing may produce a different number of regions than previously specified). To impose a fixed number of output regions, manual refinement or domain knowledge may be required, which cannot be exempt of subjectivity (Aydin et al. 2021). In geographical modelling, the number of regions is typically not known a priori. We hold that this drawback is not critical if the number of regions is not strictly constrained. We extend a common approach, K-Means algorithm, and propose an automated post-processing procedure which reduces subjectivity.

Spatially explicit methods consider spatial contiguity during the regionalization process, which ensures connectivity of regions without requiring post-processing operations. Duque et al. (2011) proposed three MIP formulations of this problem, which could be solved with commercial optimization software directly, and the optimal solution is guaranteed to be found. However, such exact methods are computationally expensive and therefore suitable to small datasets only. While heuristic methods do not guarantee to find the optimal solution, their computational advantages make

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3It would require more than three hours to solve a simulated case on a 7×7 grid. The experiments are performed using ILOG CPLEX 11.2 and executed on a computer with 8 GB of memory and a 2.99 GHz processor. See Duque et al. (2011) for further detail.
them more suitable for large datasets. Openshaw (1977) proposed the AZP algorithm, which uses an iterative process to improve an initial solution by moving a unit from one region to another while ensuring spatial contiguity. This algorithm was improved by incorporating intelligent optimization techniques, such as simulated annealing and tabu search (Openshaw and Rao 1995). Assunção et al. (2006) proposed SKATER algorithm which operates by cutting edges from the minimum spanning tree. Guo (2008) proposed REDCAP algorithm, which is a spatially explicit extension of hierarchical clustering algorithms. The latter two algorithms may produce more accurate and stable results compared to AZP (Aydin et al. 2021). As a component of PySAL, a python spatial analysis library (Rey et al. 2021), Rey developed Regional-K-Means algorithm, which uses a workflow similar to K-Means, yet checks spatial contiguity before each move. AZP offers more flexibility on the objective function, which makes it adaptable to various modelling scenarios. Regional-K-Means can be extended in a similar way with K-Means. Since SKATER and REDCAP rely on similarity measures of attributes, a generalization to model-based regionalization is not straightforward. Therefore, we consider AZP and Regional-K-Models in this study.

Unlike the aforementioned frequentist approaches, regionalization methods based on Bayesian statistics consider each parameter as a random variable, and hence, explicitly represent their uncertainty. Knorr-Held and Raßer (2000), Denison and Holmes (2001) developed Bayesian partition models to detect regions with homogeneous disease risks. Units in each partition (a contiguous region) are regarded as samples from the same distribution. The partition scheme also follows a random distribution, and the regionalization result are summarized based on samples from the posterior distribution, which combines the prior probability and information from data summarized by the likelihood. Bradley et al. (2017) proposed a two-stage regionalization algorithm to minimize a statistical criterion associated with spatial aggregation error. Teixeira et al. (2019) introduced a product partition model utilizing random spanning trees. These Bayesian methods are not suitable for regionalization within our frequentist optimization framework, hence we did not investigate their extensions.

Methods for model-based regionalization are still in the early stages of development. Bayesian mixture models such as Dirchlet processes (Ma et al. 2020) can detect clusters in regression coefficients, yet the regions produced are not necessarily contiguous (Luo et al. 2021). Li and Sang (2019) proposed the spatially clustered coefficients regression (SCC), which adopts fused lasso regularization to identify regions with similar coefficients. However, the solution space for regionalization is restricted by a predefined minimum spanning tree based on Euclidean distance, and the method may produce much more regions than expected (over-clustering) (Luo et al. 2021). Bayesian partition models can also consider the effect of covariates, yet early methods using Voronoi tessellations cannot represent latent regions of arbitrary shapes (Zhang et al. 2014). The Bayesian spatially clustered coefficient (BSCC) model (Luo et al. 2021) solves this problem by using spanning trees and therefore can be considered as a model-based regionalization algorithm.

Statistical tests may provide a rigorous framework to assess heterogeneity between regions (spatially stratified heterogeneity). Wang et al. (2016) introduced q-statistic to assess the degree of statistical significance of spatially stratified heterogeneity. Yet this

Despite that the nature of Bayesian inference is probabilistic, our taxonomy considers Bayesian methods as attribute-based if they are applied to response data only, and model-based if covariates are included, as an example.

Note that the approach from Bradley et al. (2017) is spatially implicit, while the other Bayesian approaches introduced are spatially explicit.
method considers heterogeneity of attribute values only. Adapting a similar method to model-based cases aiming at making inference on processes would require further studies and is beyond the scope of this study.

An issue closely related to regionalization is the modifiable areal unit problem (MAUP). In the context of spatial data, analytical results, such as correlation and regression coefficients, may depend on the scale and configuration of areal units (Clark and Avery 1976; Fotheringham and Wong 1991). Openshaw (1977) argues that regionalization methods may solve this problem by optimizing the set of regions; yet the optimization criteria remain subjective (Fotheringham and Wong 1991). Regionalization methods also provide tools to investigate MAUP, in the sense that extreme cases could be constructed through optimization (Openshaw and Rao 1995).

3. Framework

3.1. Geographical models

The geographical models considered in our framework can be viewed as a quantitative representation of spatial data or process, with regard to each areal unit in a spatial domain. Generally, geographic models aim at estimating parameters \( \hat{\theta} \) given a model \( \mathcal{M} \) with parameters \( \theta \in \Theta \), a dataset \( D \), and a discretized spatial domain \( D \). The dataset \( D \) includes data measured in each spatial unit \( u_i \) within \( D \). For example, in a linear regression model, \( D \) includes a dependent variable \( y_i \) and typically several features \( x_i \) measured in each \( u_i \) within \( D \). The inference process may be expressed as follows (Equation 2):

\[
\{D, \mathcal{M}(\theta), D\} \rightarrow \hat{\theta} \quad (\theta \in \Theta).
\]

Our framework can accommodate a wide range of geographic models, which may be classified into three categories:

(1) Attribute models that estimate the expected value (average) or range of plausible values in a region, with attributes only \( (D = \{y\}) \). For example, these models may estimate the annual mean precipitation or the range of plausible temperatures in a study area.

(2) Regression models describing the relationship between features and an attribute \( (D = \{x, y\}) \). For example, a linear regression model may describe the variation of gross domestic product (GDP) between countries based on two features: population size and number of enterprises.

(3) Complex geographic models used to describe geographical processes within a spatial unit. Examples include spatial interaction models between places within a spatial unit, and cellular automata for land use change.

Examples for applying our framework to the three classes of models are provided in Table 1. Attribute-based regionalization is the basic case, investigated extensively by previous studies (Duque et al. 2007, 2011; Aydin et al. 2021). Regionalized regression models aim to delineate regions with homogeneous relationship between the independent variables \( x \), and the dependent variable \( y \). The dataset \( D \) includes a dependent

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6Throughout the paper, we describe the case of lattice data (spatial data on areal units), which is common in regionalization literature. Our approach is also applicable to point observation data after building adjacency (with e.g. Delaunay triangulation).

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Table 1. Framework configuration in three typical modelling scenarios (columns 1-3)

| Component          | (1) Attribute models | (2) Regression models | (3) Complex geographic models |
|--------------------|-----------------------|-----------------------|-------------------------------|
| Data D             | \{y_i\}_{i=1}^N      | \{(x_i, y_i)\}_{i=1}^N | \{G_i\}_{i=1}^N              |
| Model M            | \mu \in \mathbb{R}^p | y = \beta x + \alpha   | g_{k,l} = cp^k p_l^k / d_{k,l}^2 |
| Error function \(\epsilon\) | \|y_i - \mu\|^2_2    | (\beta x_i + \alpha - y_i)^2 | \sum_{k,l}(h_{k,l} - cp^k p_l^k / d_{k,l}^2)^2 |
| Fitting method f   | Mean                  | OLS                   | OLS or simulated annealing    |

variable \(y_i\) and a independent vector \(x_i\) for each unit, with parameters composed of an intercept \(\alpha_j\) and a coefficient vector \(\beta_j\) that may vary across regions. We further investigate this scenario in Section 4. Our framework is applicable to the zone design problem related to a variety of complex geographic models as well. As an example, we discuss the gravity model for spatial interactions in Section 5.

Note that we exclude models which are only applied to an entire region (composed of a set of spatial units), rather than considering each spatial unit in a region. An example is global auto-correlation statistics applied to spatial cross-sectional data, which computes a unique aggregated value for each region. For similar reasons, we do not consider spatial interaction models between spatial units either.

3.2. Framework overview

Our framework aims at jointly estimate the regional parameters \(\theta\) of a geographic model \(M\), denoted as \(\theta = \{\theta_j\}_{j=1}^\gamma\), along with the number of regions \(\gamma\) and the delineation of regions \(R = \{R_j\}_{j=1}^\gamma\) within a study domain \(D\). The input of the framework includes: a set of areal units \(\{u_i\}_{i=1}^N\), a dataset \(D\) with values provided for each areal unit, and a geographic model \(M\) with parameters \(\theta\) that are allowed to vary across the regions within \(D\). During the optimization process, the spatial areal units \(\{u_i\}_{i=1}^N\) are aggregated into spatially connected regions \(\{R_j\}_{j=1}^\gamma\), so that optimal parameter values and regions are obtained. Note that \(D\) and \(\theta\) may represent various quantities according to different modelling settings (Table 1). The inference process of the proposed framework may be expressed as follows (Equation 3):

\[
\{D, M(\theta), D\} \rightarrow \{R_j, \hat{\theta}_j\}_{j=1}^\gamma (\theta_j \in \Theta).
\]

Figure 1 provides an overview of the proposed framework. The analytical procedure includes three major steps: model selection, objective function definition, and optimization. In the model selection step, a model \(M(\theta)\) is specified, together with a parameter space \(\Theta\), which defines the possible values of the model parameters. A corresponding fitting algorithm \(f\) is required, which is the calibration algorithm for \(M(\theta)\) in the general case. It is used to estimate and update the regional parameters in the regionalization process. To combine both the model’s accuracy and ability to reconstruct the regions, we include two terms in the objective function: (a) an error term measuring the discrepancies between the model predictions and the observations.

\[7\] In our framework, we specify a class of model from which parameters will be estimated. Note that for a given class of models, the number of parameters are allowed to vary according to dynamic changes in the number of regions during the optimization process.
and (b) a penalty term used to favor parsimonious models. We investigate and compare three optimization algorithms to optimize the regionalization scheme, including two spatially explicit and one spatially implicit algorithms.

### 3.3. Objective function

In our framework, the determination of an optimal number $\gamma$ and the delineation of regions are constrained to account for the trade-off between the accuracy and the generality of the model. Note that accuracy is obtained when the model output is close to the observation data, and generality is obtained when a set of parameters is applied to a large area, rather than a specific location. While allowing the model parameters to vary for each spatial unit within a domain would maximize accuracy and potentially eliminate modelling errors, each set of parameters would only be applicable to its corresponding spatial unit. On the other extreme, forcing the parameters to be invariant across the whole spatial domain would maximize the model’s generality, yet it would not be able to reveal potential heterogeneity between regions within the domain. Hence, jointly learning the optimal number of regions and their delineation while estimating model parameters may lead to the identification of an optimal solution that accounts for both model accuracy and generality. In our framework, this is obtained by minimizing the following objective function (Equation 4):

$$L(R, \theta) = E(y, \hat{y}) + \lambda C(R),$$

(4)

where $E$ stands for inductive error, which is a function measuring the total error between the model predictions $\hat{y}$ and the observed data $y$. $C$ stands for complexity, a function measuring the complexity of the regionalization scheme $R = \{R_j\}_{j=1}^\gamma$. We set $C(R) = \gamma$ to penalize solutions proportionally to the number of output regions. To allow different penalty levels associated with the complexity, we introduced the hyperparameter $\lambda$. A higher value of $\lambda$ favors simpler solutions, and hence, tends to produce less regions.

More specifically, the inductive error $E$ is the sum of the modelling errors $\epsilon(\cdot)$ com-

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8Our framework could have incorporated other complexity elements such as perimeter or compactness of regions. However, to make our framework as general as possible, we favored a simple formulation for region complexity, i.e. the number of regions, which can be applicable in all considered geographical models without additional adjustments.
puted in each spatial unit \( u_i \), with \( i = 1, \ldots, N \) (Equation 5):

\[
\mathcal{E}(\mathbf{y}, \hat{\mathbf{y}}) = \sum_{i=1}^{N} \sum_{j=1}^{\gamma} I[u_i \in R_j] \epsilon(\hat{y}_{i,j}, y_i),
\]

where \( y_i \) is data observed at \( u_i \); \( \hat{y}_{i,j} \) is the model prediction at \( u_i \) with parameters \( \theta_j \). The function \( \epsilon \) measures the local modelling error in a spatial unit. A fitting algorithm \( f \) is used to estimate the model parameters \( \hat{\theta}_j \) used in region \( R_j \), which can be expressed as follows (Equation 6):

\[
\hat{\theta}_j = \arg \min_{\theta_j \in \Theta} \sum_{i=1}^{N} I[u_i \in R_j] \epsilon(\hat{y}_{i,j}, y_i).
\]

In attribute-based regionalization, we have \( \epsilon(\hat{y}_{i,j}, y_i) = \| y_i - \mu_j \|^2 \). The form of the error \( \mathcal{E} \) is the same with the objective function in generic clustering analysis\(^9\). The mean vector of attributes

\[
\mu_j = \frac{1}{|R_j|} \sum_{i=1}^{N} I[u_i \in R_j] y_i
\]

is the exact solution of Equation 6. In the case of regionalized regression, we have \( \epsilon(\hat{y}_{i,j}, y_i) = (y_i - \beta_j x_i + \alpha_j)^2 \). The linear models are calibrated through ordinary least squares estimation (OLS), which minimizes the sum of squared errors (Table 1).

### 3.4. Optimization algorithms

We compare the performance of three algorithms to optimize the objective function and reconstruct the regions. This includes two spatially explicit algorithms, AZP and Regional-K-Models, and one spatially implicit algorithm, K-Models (with post-processing). All considered algorithms start with an initial feasible solution and execute an iterative process to find an optimal solution. In K-Models and Regional-K-Models, a unit can only be moved into the region with its “closest” model (i.e. the model with the lowest residual). However, in AZP, a move is allowed as long as it decreases the objective function value.

#### 3.4.1. K-Models with post-processing

We introduce K-Models as an extension of the classical K-Means clustering algorithm (MacQueen [1967]). In the K-Models algorithm, we associate each region with a set of model parameters, which takes the role of cluster centers in K-Means. A cluster center is described by the mean vector, a set of model parameters in \( \mathbb{R}^p \), where \( p \) is the number of features. Thus, K-Means is a special case of K-Models.

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\(^9\)Note that the observed data \( x_i \) and \( y_i \) associated with \( u_i \) can be vectors rather than scalars. We describe the scalar case to simplify the notation. Generalizing the equations and algorithms to vector objects is straightforward.

\(^{10}\)Note that in Equation 1, the number of considered unit pairs in the sum is \( \sum_{j=1}^{M} (|R_j|) \), which is smaller if \( |R_j| (j = 1, \ldots, M) \) are close to each other. Hence that objective function might favor solutions whose regions have similar numbers of units, while the objective function used here does not suffer from this issue.
Algorithm 1 K-Models

**Input:** Domain $\mathcal{D}$ composed of spatial units $\{u_i\}_{i=1}^N$; data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$; number of regions $K$; maximum iterations $L$.

**Output:** Regions $\{\mathcal{R}_j\}_{j=1}^K$ and estimated parameters $\{\hat{\theta}_j\}_{j=1}^K$.

1. Generate initial regions $\{\mathcal{R}_j\}_{j=1}^K$ and estimate initial parameters $\{\hat{\theta}_j\}_{j=1}^K$;
2. stable = False;
3. $t = 0$;
4. while not stable and $t < L$ do
5.   $\mathcal{R}'_j = \emptyset$, $j = 1, 2, \ldots, K$;
6.   for $i = 1, 2, \ldots, N$ do
7.     Identify the region whose parameters fit $(x_i, y_i)$ best: $r_i = \arg \min_j \epsilon(y_i, \hat{y}_{i,j})$;
8.     Add $u_i$ to the region with the lowest error at $u_i$: $\mathcal{R}'_{r_i} = \mathcal{R}'_{r_i} \cup \{u_i\}$.
9.   for $j = 1, 2, \ldots, K$ do
10.    Estimate the model parameters: $\hat{\theta}'_j = \arg \min_{\theta_j \in \Theta} \sum_{i=1}^N I[u_i \in \mathcal{R}'_j] \epsilon(y_i, \hat{y}_{i,j})$;
11.   if $\mathcal{R}_j = \mathcal{R}'_j$, with $j = 1, 2, \ldots, K$ then
12.      stable = True
13.   Update regions and parameters: $(\mathcal{R}_j, \hat{\theta}_j) = (\mathcal{R}'_j, \hat{\theta}'_j)$, with $j = 1, 2, \ldots, K$;
14.   $t = t + 1$;
15. return $\{\mathcal{R}_j, \hat{\theta}_j\}_{j=1}^K$.

The K-Models algorithm starts with a randomly generated initial regionalization scheme with $K$ regions. For each initial region $\mathcal{R}_j$, a set of model parameters $\theta_j$ is initialized using the fitting algorithm $f$. Each iteration includes two steps. First, for each spatial unit, the error of each regional model is calculated, and the unit is moved to the region whose model fits it best. Second, the model parameters of each region are updated with $f$, as units are moved into or out of the region in the first step. The algorithm stops if no unit is moved during an iteration, or when the maximum number of iterations is reached. Note that the objective function value is non-increasing in both steps. The pseudo code for this algorithm is in Algorithm 1.

To generate the initial solution, $K$ random seeds are picked from $\{u_i\}_{i=1}^N$. Next, for each region, if it has unassigned neighboring units, one of them is randomly chosen and assigned to the region. This procedure is repeated until every unit is assigned to a region. This method ensures the spatial contiguity of each region.

The resulting regions from the K-Models procedure are not necessarily connected. A post-processing procedure is introduced to ensure the connectivity of each region, as well as improve the solution. First, if a region is disconnected, it is divided into connected branches. A new set of model parameters is fitted for each branch. After this step, the number of regions may be larger than $K$. Second, we examine each pair of neighboring regions, and calculate changes in the objective function if they are merged (a new set of model parameters is fitted for the merged region). The pair of regions that produces the largest decrease of the objective function value are merged into one region. This procedure is repeated until no additional decrease in the objective function value can be obtained by merging two neighboring regions. The idea of merging after partitioning is inspired by two-stage clustering algorithms such as Chameleon [11].

Unlike spatially explicit AZP and Regional-K-Models, K-Models does not require the initial regions to be geographically connected. This setting is a reflection of Tobler’s law that neighboring units tend to be similar.

11 Unlike spatially explicit AZP and Regional-K-Models, K-Models does not require the initial regions to be geographically connected. This setting is a reflection of Tobler’s law that neighboring units tend to be similar.
Algorithm 2 AZP

\textbf{Input:} Domain \( D \) composed of spatial units \( \{u_i\}_{i=1}^N \); data \( D = \{(x_i, y_i)\}_{i=1}^N \); number of regions \( K \).

\textbf{Output:} Regions \( \{R_j\}_{j=1}^K \) and estimated parameters \( \{\hat{\theta}_j\}_{j=1}^K \).

1: Generate initial regions \( \{R_j\}_{j=1}^K \) and estimate initial parameters \( \{\hat{\theta}_j\}_{j=1}^K \);
2: stable = False;
3: \textbf{while} not stable \textbf{do}
4: stable = True;
5: for \( j = 1, 2, \cdots, K \) \textbf{do}
6: \( P = \emptyset \);
7: for \( v \) in the set of units which are connected with \( R_j \) \textbf{do}
8: \text{Find the region } \( R_d \) such that \( v \in R_d \);
9: \text{if } \( R_d \setminus \{v\} \) is connected and moving \( v \) to \( R_j \) decreases the value of the objective function \textbf{then}
10: \( P = P \cup \{v\} \);
11: \textbf{if } \( P \neq \emptyset \) \textbf{then}
12: stable = False;
13: \text{Randomly choose } v \in P ;
14: \text{Move } v \text{ into } R_j \text{, and update the model parameters.}
15: \textbf{return } \{R_j, \theta_j\}_{j=1}^K.

Similar with K-Means, a parameter \( K \) is required as input. However, due to the merging procedure, it is \( \lambda \), rather than \( K \), that largely determines the number of regions produced. As long as \( K \) is not too small, the algorithm is able to produce regions with reasonable sizes. One can further improve the solution by exploring different values of \( K \). In rare cases, the K-Models algorithm may produce an empty region in the process. Such cases are more frequent if \( N \gg K \) does not hold. A simple remedy to this issue is to delete the empty region, as the parameter \( K \) does not actually restrict the number of final output regions.

3.4.2. AZP

Of the three algorithms, AZP is the most flexible in terms of the form of the objective function. If the function \( \mathcal{E}(y, \hat{y}) \) is not in the form of Equation 5, AZP is still applicable, while the other two algorithms based on K-Means are not. Using the same method applied in K-Models, an initial solution is generated, which satisfies the spatial contiguity constraint. Subsequently, AZP tries to improve the solution by moving a region’s neighboring unit into the region. A unit is neighbor of a region if their boundary share a common edge. The AZP procedure is described in Algorithm 2.

Two conditions need to be met to allow moving a unit from one region to another: (a) the donor region remains connected after giving out the unit; (b) the move leads to a decrease in the objective function value. The first condition involves the verification of graph connectivity. A breadth-first search approach has a time complexity of \( O(|E|) \), where \( E \) is the set of edges in the adjacent graph. Assessing the validity of the second condition for spatial unit \( v \) in the neighborhood of \( R_j \) requires fitting new models for \( \mathcal{R}_j \cup \{v\} \) and \( \mathcal{R}_d \setminus \{v\} \). For attribute models such as mean vectors, the time complexity is \( O(N) \). Yet it would require much more operations to fit the models in a linear regression.
### Algorithm 3 Regional-K-Models

**Input:** Domain $D$ composed of spatial units $\{u_i\}_{i=1}^N$; data $D = \{(x_i, y_i)\}_{i=1}^N$; number of regions $K$.

**Output:** Regions $\{R_j\}_{j=1}^K$ and estimated parameters $\{\hat{\theta}_j\}_{j=1}^K$.

1. Generate initial regions $\{R_j\}_{j=1}^K$ and estimate initial parameters $\{\hat{\theta}_j\}_{j=1}^K$;
2. stable = False;
3. while not stable do
4.   stable = True;
5.   $P = \emptyset$;
6.   for $i = 1, 2, \ldots, N$ do
7.     Identify the region $R_{d_i}$ that contains $u_i$;
8.     Identify the region $R_{r_i}$ with the lowest local error: $r_i = \arg\min_j \epsilon(y_i, \hat{y}_{i,j})$;
9.     if $d_i \neq r_i$ and $R_{d_i} \setminus \{u_i\}$ and $R_{r_i} \cup \{u_i\}$ is connected then
10.    $P = P \cup \{u_i\}$;
11.   if $P \neq \emptyset$ then
12.      stable = False;
13.      Randomly choose $u_i \in P$;
14.      Move $u_i$ into $R_{r_i}$, and update the related model parameters.
15. return $\{R_j, \theta_j\}_{j=1}^K$.

setting. The less computationally expensive condition should be verified first, which depends on the modelling scenario. In the presence of two or more valid neighboring units of $R_j$, only one unit is moved, as it may affect the validity of subsequent moves. Figure 2a illustrates the potential issues associated with simultaneous moves.

Unless an empty region is produced during the process, the output of AZP consists of exactly $K$ regions. As a result, if $C(R) = \gamma$, the parameter $\lambda$ does not play a role during the process (Equation 4). Hence, it is necessary to search different $K$ values to identify the best solution.

### 3.4.3. Regional-K-Models

We propose to extend Regional-K-Means algorithm (Feng et al. 2021), which is further referred to as Regional-K-Models. In contrast to the K-Models algorithm, spatial contiguity is checked before each move, which makes Regional-K-Models spatially explicit. The procedure of Regional-K-Models is described in Algorithm 3. Similar with K-Models, the objective function is non-increasing in both unit moving and model updating.

As a unit is allowed to be moved into its neighboring region with the best model fit only, the range of potential candidate moves is rather restricted compared with AZP. Similar to AZP, only one candidate move is performed at a time, in order to prevent potential break of the contiguity constraint induced by simultaneous moves (see illustrated example in Figure 2b), and different values of $K$ are investigated to find the optimal solution.

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Figure 2. Examples of spatial contiguity breaks that may occur if two moves are performed simultaneously. (a) $R_1$, $R_2$ are regions, and units $u_1$, $u_2$ initially belong to $R_2$. In AZP algorithm, moving $u_1$ or $u_2$ into $R_1$ satisfies the contiguity constraint, while moving both of them into $R_1$ simultaneously makes $R_2$ disconnected. (b) In Regional-K-Models, a similar situation may occur for region $R_4$, if $v_1$ is moved into region $R_3$, and simultaneously, $v_2$ is moved into $R_5$, although either move is in principle valid.

4. Application in spatial regression scenarios

To assess the validity and usefulness of the proposed regionalization framework, we performed a set of experiments within a spatial regression context. Spatial regression models allow identifying and quantifying effects of features on a response, while accounting for spatial dependency in the data. Spatial lag models (SLM, Anselin (2010)) and geographically weighted regression (GWR, Brunsdon et al. (1996)) are two common approaches. SLM is a family of global regression models which incorporate spatial lag effects to account for spatial dependency within a neighborhood. GWR is a local regression approach, modelling spatial heterogeneity by allowing parameters to vary across space. The suggested framework provides an approach complementary to SLM and GWR, including a regionalization process and a set of linear regression coefficients calibrated for each region. We term it **regionalized regression**, which is at the midpoint between global and local regression. It is a special case of multilevel linear regression (Gelman and Hill 2007), where data are divided into groups, and coefficients are allowed to vary for different groups. In regionalized regression, each group stands for a geographically connected region. Moreover, the Bayesian spatially clustered coefficient model (BSCC) is similar in intent to our frequentist approach.

Note that regionalized regression can be performed using the framework of GWR as well. For each spatial unit, GWR estimates a set of linear regression coefficients. Thus, an attribute-based regionalization can be applied to the estimated local coefficients, and produce connected regions with a similar relationship between variables. In this GWR approach, the estimation of the regression coefficients and region delineation are optimized separately. On the contrary, the proposed framework jointly optimizes region delineation along with the regression coefficients, which can lead to better optimization and region reconstruction performance.

We performed linear regression experiments on two synthetic datasets, as well as real data gathered from the Georgia open dataset (Yu et al. 2020). We implement and test all three algorithms of our framework and included the GWR method as benchmark.

4.1. Simulation design

Simulated data experiments are performed on a $25 \times 25$ regular grid, where each grid cell represents a spatial unit. For each cell, each independent variable $x_i$ is generated from an independent uniform distribution in $[0, 1)$; the dependent variable $y$ is generated from a uniform distribution in $[0, 1)$.
Figure 3. Three examples of the parameter surface of $\beta_1$ in Dataset 1. In each simulation, the parameter surface is generated by Voronoi polygons of five random seed points. Each polygon is assigned a different value of $\beta_1$.

erated from a linear model, with predefined linear coefficients. Rook contiguity (cells sharing a side are considered neighbors) is used in all simulations. We simulate two datasets (Dataset 1 and Dataset 2).

In Dataset 1, the relationship between $x$ and $y$ exhibits a strict stratified heterogeneity. That is, the linear coefficients are identical in each predefined region, and distinct in different regions. This simulation aims to test whether our framework can reconstruct the underlying regions associated with geographical processes, given the spatial distributions of $x$ and $y$. The data generating process can be expressed as follows (Equation 8):

$$y = \beta_0 + \beta_1 x + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$

where $x \sim U(0, 1)$, $\beta_0 \equiv 0$, and the errors follow a normal distribution with mean 0 and variance $\sigma^2$. Five cells are randomly picked as seed points, and their corresponding Voronoi polygons produce five spatially connected regions $R_1, \ldots, R_5$. The covariate coefficient $\beta_1$ are set as -2, -1, 0, 1, 2 in region $R_1, \ldots, \text{and} R_5$, respectively (Figure 3).

In Dataset 2, the relationship between $x$ and $y$ varies continuously across space. This dataset mimics a real case scenario that is common in environmental sciences, where the change in model parameters is gradual across region boundaries, instead of the abrupt changes between regions in Dataset 1. The data generating process of Dataset 2 can be expressed as follows (Equation 9):

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$

where $x_1, x_2 \sim U(0, 1)$. The linear coefficients are set to express distinct levels of heterogeneity (Fotheringham et al. 2017),

$$\beta_0 = 0$$

$$\beta_1 = \frac{1}{24}(r + c) - 1$$

$$\beta_2 = \cos(\pi e^r/22) \cos(\pi e^c/22)$$

where $r, c$ are row and column numbers in the grid (from 0 to 24), respectively. The
parameter surfaces are illustrated in Figure 4. In this setting, $\beta_0$ is constant across space, with no heterogeneity. $\beta_1$ shows a slope across space, with a maximum of 1 and a minimum of -1 at two opposite corners of the grid. $\beta_2$ shows a high level of heterogeneity, with five high value areas (peaks) and four low value areas (valleys). The variability of the sizes of peaks and valleys are designed to assess the ability of our approach to reconstruct regions of different sizes driven by heterogeneous processes with spatially varying scales (Fotheringham and Sachdeva 2022).

Using the data generating processes defined above, we produced a set of samples for both datasets. For Dataset 1, we set different values of $\sigma$ to evaluate the effect of random noise on regionalization. Three conditions are considered, namely low noise ($\sigma = 0.1$), medium noise ($\sigma = 0.2$), and high noise ($\sigma = 0.3$). 50 parameter surfaces are simulated, and three $x,y$ arrays are generated for each parameter surface, using different noise levels. $\lambda = 5$ is used for Dataset 1. For Dataset 2, with the parameter surfaces defined above, 50 sets of $x,y$ arrays are simulated. We test the cases where $\lambda = 5$ and $\lambda = 3$, representing different regionalization scales. We assume low noise ($\sigma = 0.1$).

In this study we consider model complexity as the number of output regions. We run each algorithm with parameter $K$ that varies from 2 to 20 (except that for GWR, we considered $K$ from 2 to 60 since it appears to produce better results with values of $K > 20$), and select the solution that show the lowest objective function value. For GWR, the derived local coefficients are regionalized with K-Means (the basic case of K-Models) and post-processing, as described in Section 3.4.1. GWR applies an adaptive bisquare kernel with corrected Akaike information criterion (AICc) used as criterion to select the bandwidth (Fotheringham et al. 2017).

To compare the optimization performance of the considered algorithms, we report the objective function values. To assess the ability of the algorithms to reconstruct the latent regions, we compute the Rand index (RI) and the normalized mutual information (NMI) for experiments on Dataset 1. Such metrics are not applicable for Dataset 2 since there are no distinct underlying regions. We visually compare the delineated regions with latent parameter surfaces and check if the algorithms produce reasonable

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12We consider different noise conditions only in the experiments on Dataset 1. Obtaining distinct latent regions ease the assessment of regionalization performance.

13Note that GWR can be combined with other attribute-based regionalization algorithms such as AZP, SKATER and REDCAP. We use K-Means here to compare the results with the K-Models approach.
Figure 5. Four possible situations for a pair of spatial units in the calculation of RI. $\mathcal{R}_1$, $\mathcal{R}_2$ are true regions, $\mathcal{R}_1'$, $\mathcal{R}_2'$ are reconstructed regions, $u_i (i = 1, 2, 3, 4)$ are units. $(u_3, u_4)$ is a true positive (TP) pair, $(u_1, u_2)$ is a false negative (FN) pair, $(u_2, u_3), (u_2, u_4)$ are two false positive (FP) pairs, $(u_1, u_3), (u_1, u_4)$ are two true negative (TN) pairs.

There are four possible situations for each pair of spatial units in a regionalization result (Figure 5):

- **True positive (TP):** two units are in the same region for both the true region scheme and the reconstructed region scheme.
- **False negative (FN):** two units are in the same region in the true result, but mistakenly grouped into different regions by the algorithm.
- **False positive (FP):** two units are in different regions in the true result, but mistakenly grouped into the same region by the algorithm.
- **True negative (TN):** two units are in different regions for both the true region scheme and the reconstructed region scheme.

RI (Rand 1971) calculates the proportion of correctly grouped pairs of units as follows (Equation 13):

$$RI = \frac{TP + TN}{TP + FN + FP + TN}. \quad (13)$$

RI can take value between 0 and 1. Higher values indicate a better region reconstruction. RI takes the value 1 if all reconstructed regions are identical to the true regions.

NMI measures the difference of two region schemes from an information theory perspective (Vinh et al. 2010). Assume $\mathcal{R} = \{\mathcal{R}_j\}_{j=1}^M$ are the true underlying regions, and $\mathcal{R}' = \{\mathcal{R}_j\}'_{j=1}^M$ are reconstructed regions. The entropy $H(\mathcal{R})$ is defined as follows (Equation 14):

$$H(\mathcal{R}) = -\sum_{j=1}^M \frac{|\mathcal{R}_j|}{N} \log \frac{|\mathcal{R}_j|}{N}, \quad (14)$$

where $N$ is the total number of units. The mutual information $(I(\mathcal{R}, \mathcal{R}'))$ of $\mathcal{R}$ and $\mathcal{R}'$ is calculated as follows:

$$I(\mathcal{R}, \mathcal{R}') = \sum_{j=1}^M \frac{|\mathcal{R}_j|}{N} \log \frac{|\mathcal{R}_j|}{N}.$$


Table 2. Mean objective values obtained from 50 simulations on two simulated datasets.

| Algorithm           | Dataset 1          |                      | Dataset 2          |                      |
|---------------------|--------------------|----------------------|--------------------|----------------------|
|                     | Low noise | Medium noise | High noise | $\lambda = 5$ | $\lambda = 3$ |
| K-Models             | 31.05      | 49.42          | 79.32          | 50.25             | 40.10             |
| AZP                 | 59.60      | 87.26          | 120.10         | 58.14             | 48.89             |
| Regional-K-Models   | 83.23      | 125.53         | 161.78         | 62.95             | 56.73             |
| GWR                 | 41.73      | 60.18          | 89.48          | 51.34             | 41.97             |

Note: Noise levels stand for variance of the error term in the linear model. Low noise: $\sigma = 0.1$; medium noise: $\sigma = 0.2$; high noise: $\sigma = 0.3$. We set $\lambda = 5$ for Dataset 1, and $\sigma = 0.1$ for Dataset 2. The lowest objective function value in each simulation setting is put in bold.

$R'$ is defined as follows (Equation 15):

$$I(R, R') = \sum_{j=1}^{M} \sum_{k=1}^{\gamma} \frac{|R_j \cap R'_k|}{N} \log \frac{N|R_j \cap R'_k|}{|R_j||R'_k|}. \quad (15)$$

Based on the concepts above, NMI can be expressed as follows (Equation 16):

$$\text{NMI}(R, R') = \frac{I(R, R')}{H(R)H(R')} \quad (16)$$

The range of NMI is $[0,1]$. High NMI values indicate that one region scheme provides a large amount of information for the other, which suggests similarity between the two region schemes.

All experiments are performed on a computer with dual Intel Xeon Gold 5118 CPUs (2.30GHz) and 256GB of memory. The data generating process and regionalization algorithms are implemented in Python 3.9, utilizing the NumPy package [Harris et al. 2020]. We use the linear regression API provided by scikit-learn [Pedregosa et al. 2011]. Libpyosal and mgwr [Oshan et al. 2019] modules in PySAL [Rey et al. 2021] are used as well for handling spatial weights and performing GWR, respectively.

4.2. **Results**

Table 2 shows the mean objective function values of the four algorithms associated with Dataset 1 and Dataset 2. For Dataset 1, the spatially implicit method, K-Models, shows a relatively good overall performance compared to the two spatially explicit methods, AZP and Regional-K-Models. K-Models achieves the best performance in all 150 test cases (50 simulations, each with three noise levels). As for GWR combined with K-Means, which is also a spatial implicit approach, it outperforms AZP and Regional-K-Models as well, yet shows a lower performance compared to K-Models. Table 3 shows the mean RI and NMI values for 50 simulations in Dataset 1. For all algorithms, both RI and NMI decreases as the noise level increases. K-Models achieves the best result for both metrics, regardless of the noise level. Regarding region reconstruction, the performance of AZP and Regional-K-Models is still not as good as GWR.

Figure 6 illustrates the regionalization results of a simulation from Dataset 1. Both K-Models and GWR are able to reconstruct relatively well the spatial distribution of the parameter values. As the noise level increases, the regionalization results show a slight discrepancy at the region boundaries, yet the general pattern remains correctly reconstructed. AZP and Regional-K-Models tend to produce regions with more
Table 3. Mean values of Rand index (RI) and normalized mutual information (NMI) obtained from 50 simulations on Dataset 1.

| Algorithm        | Low noise | Medium noise | High Noise |
|------------------|-----------|--------------|------------|
|                  | RI        | NMI          | RI         | NMI        | RI         | NMI        |
| K-Models         | 0.9891    | 0.9551       | 0.9757     | 0.9128     | 0.9616     | 0.8728     |
| AZP              | 0.8715    | 0.7361       | 0.8399     | 0.6578     | 0.8211     | 0.6095     |
| Regional-K-Models| 0.8559    | 0.6784       | 0.8079     | 0.5752     | 0.8011     | 0.5569     |
| GWR              | 0.9676    | 0.8802       | 0.9620     | 0.8644     | 0.9538     | 0.8399     |

Note: In each simulation setting, the highest RI and NMI values are put in bold. Low noise: $\sigma = 0.1$; medium noise: $\sigma = 0.2$; high noise: $\sigma = 0.3$.

branches, which are deviations from the true parameter surface. This suggests that spatially explicit methods may have a disadvantage in a regionalized regression setting. For spatially explicit methods, the options to improve the results are restricted by the contiguity constraint, which may lead to a sub-optimal result. Moreover, both algorithms seem to be affected by large random noise in the linear model.

For Dataset 2, the performance rank of the four algorithms, measured by the objective function, is similar to the results on Dataset 1. K-Models achieves the best result in 76% of the simulations (38 out of 50) when $\lambda = 5$, and in 92% of the simulations (46 out of 50) when $\lambda = 3$. GWR performs best in all but one of the remaining simulations. K-Models shows the best overall result, yet the improvement compared to GWR is marginal. Spatial explicit approaches, AZP and Regional-K-Models show a lower overall performance. Figure 7 shows the regionalization results of an illustrative simulation for $\lambda = 5$ and $\lambda = 3$. The reconstructed regions appear jointly affected by the spatial variation of the coefficients $\beta_1$ and $\beta_2$. All algorithms tend to delineate less regions in the case when $\lambda = 5$, as a large $\lambda$ value corresponds to a higher penalty associated with the number of regions. K-Models and GWR seem to generate sensible results, reflected by an increase in $\beta_1$ from the top left to the bottom right of the grid. Furthermore, they reconstruct larger peaks and valleys while ignoring smaller ones, which reflects parsimony. AZP and Regional-K-Models generate undesirable branches. Moreover, Regional-K-Models often produces solutions with only two or three regions, indicating that the algorithm fails to find a better result for larger $K$ values. This might be due to more limited candidate moves in Regional-K-Models compared to AZP.

The results demonstrate the ability of the proposed framework to reconstruct latent homogeneous regions related to geographical processes. In the spatial regression scenario, the K-Models algorithm shows the best performance, outperforming the baseline method of GWR with attribute-based regionalization, as well as two spatially explicit methods. The processes involved in the algorithms include some degree of randomness. A different region initialization may affect the optimization result. The order in which algorithms execute checks throughout all regions or units may lead to different reconstructed regions for the same dataset. In practice, repeated runs could be performed to identify more systematically the best optimization result. It requires about ten minutes to half an hour on our machine to regionalize a $25 \times 25$ grid in the experiment above.

We provide detailed results on the algorithm stability and running time in Appendix A. Appendix B provides further discussion on the choice of the hyperparameter $\lambda$ and the effect of changes in $K$ values.
Figure 6. Regionalization results of one illustrative simulation in Dataset 1. The first row shows the true parameter surface of $\beta_1$. Other rows show the estimated spatial distributions of $\beta_1$ from four algorithms (K-Models, AZP, Regional-K-Models, and GWR). Cells in each region have the same coefficient value. The columns show noise levels used in different experiments. Low noise: $\sigma = 0.1$; medium noise: $\sigma = 0.2$; high noise: $\sigma = 0.3$. 
Figure 7. Regionalization results of one illustrative simulation in Dataset 2. The first row shows the true parameter surface of $\beta_0, \beta_1, \beta_2$, respectively. Other rows show the estimated spatial distributions of the parameters from four algorithms (K-Models, AZP, Regional-K-Models, and GWR). Each panel shows different values of $\lambda$, with (a) $\lambda = 5$; (b) $\lambda = 3$. 
4.3. An empirical example

We performed regionalized regression on the Georgia open dataset, a sample dataset from the mgwr software (Oshan et al., 2019). This dataset has been used in previous spatial regression studies (e.g., Fotheringham et al. (2002), Griffith (2008), Yu et al. (2020)). The data are collected from a population census in 1990 and include socio-economic attributes of 159 counties in Georgia, USA (Oshan et al., 2019). We consider the regression of the percentage of people with a bachelor’s degree or higher (PctBach), with intercept and explanatory variables including the percentage of people born in a foreign country (PctFB), the percentage of African American (PctBlack), and the percentage of rural residents (PctRural). To ease comparison of the results with those from GWR, we use the same explanatory variables as in Yu et al. (2020).

We compare the three algorithms from the proposed framework, as well as GWR. We set \( C(R) = \gamma \), with \( \gamma \) the number of output regions and \( \lambda = 3 \). We search a set of \( K \) values identical to those used in the experiments on simulated data above. Each algorithm is repeated 10 times to obtain better optimization results. The results show that K-Models achieves the lowest objective function value, followed by GWR and AZP (Figure 8). We observe that all three algorithms show a general discrepancy along the north-south axis. The overall performance of Regional-K-Models is mediocre, as illustrated by the highest objective function value obtained among the four algorithms.

We focus on the result of the K-Models algorithm, which is the best solution according to the objective function values. Figure 9 shows the estimated coefficients on standardized data for each region. We observe an outlier region with only 2 units (counties), where the number of units is less than the number of linear coefficients. In this case, the algorithm uses the minimal-norm solution of normal equations in OLS estimation, yet it does not suffice to produce reliable coefficient estimates. In the other three regions, an overall F-test of the regional regression model appears significant at 1% level. The effect of foreign born residents is positive, and slightly higher in the northern area. Rural residents has a negative effect across Georgia. The effect of African American is positive in the north, and negative in the south. Generally, these results are consistent with the results from GWR (Yu et al., 2020). Compared with GWR, our approach successfully detects the general pattern of coefficient variation, while capturing regional heterogeneity between three regions (along with one outlier).

\footnote{Note that predicted percentages should be within 0 and 100%. All local predictions of the four results were within this range, so no truncation was needed in the experiments.}
5. Discussion and conclusions

Regional modelling is a promising approach that accounts for both spatial heterogeneity and dependency, while finding an equilibrium between optimizing generality and accuracy of geographical models. Our generalized framework provides an approach to jointly delineate regions and make inference on processes underlying geographic phenomena beyond descriptive approaches that would focus on the form (Goodchild 2004, Fotheringham and Sachdeva 2022). Building on three existing regionalization algorithms, we extend their functionality to identify homogeneous regions given a class of models. The extended spatial optimization heuristics provide an alternative methodology to spatially clustered coefficient models based on Bayesian statistics. Instead of specifying a fixed region number $K$, we added a parameter $\lambda$ to favor parsimonious models while providing some flexibility in the way model complexity is penalized. This also enables the use of spatial implicit regionalization algorithms.

Along with clustering and regression settings, our proposed framework is readily applicable to a wide range of geographic models. For example, the general gravity model (Getis 1991) is used to predict the spatial interaction flow between two places (Equation 17):

$$g_{k,l} = \frac{p_k^a p_l^b}{d_{k,l}^c \omega},$$

(17)

where $g_{k,l}$ is the estimated flow from place $k$ to place $l$; $p_k, p_l$ are place sizes, represented by population or GDP, for example; $d_{k,l}$ is the distance between $k$ and $l$; $a, b, c, \omega$ are model parameters. The gravity model can be calibrated for each spatial unit $u_i$, if a local interaction network $G_i$ (a directed graph whose nodes are places in the unit, and the edge weight from node $k$ to $l$ is the observed interaction flow $h_{k,l}$) is known. In this case, our framework can aggregate units with similar model parameters, and finally produce a regionalization scheme, with each region equipped with a set of parameters $\theta = \{a, b, c, \omega\}$ (see Table 1). The gravity model can be calibrated with OLS after a logarithm transformation, or using an intelligent optimization method such as simulated annealing (Kirkpartick et al. 1983). Other complex models such as cellular automata or neural-network-based remote sensing image classifiers may be accommodated into our framework in a similar way. They may require specific fitting
algorithms such as stochastic gradient descent for neural networks.

Spatial implicit methods for regionalization have been largely overlooked by the literature. Within a regression context, our results show that when the number of regions was not strictly restricted, the spatially implicit K-Models approach better reconstructed the regions both on simulated and real data. This approach offers a wider range of improving moves during iteration, by relaxing the requirements on region connectivity. Afterwards, a post-processing procedure would merge redundant regions and ensure spatial contiguity in the final results. While our experiments illustrate the potential of our framework, future work would be required to carry out a comprehensive algorithm comparison, including the Bayesian approach BSCC. Furthermore, more work may be carried out to examine the performance of K-Models in attribute-based regionalization, regionalization for process modelling, and on data with different sizes and generating processes.

In many cases, the calibration of regional models imposes a lower bound on the number of units in a region. In attribute-based regionalization, a region with only one or two units is not problematic. However, in the experiment on the Georgia dataset, at least four units are required to estimate regression coefficients and more units would be necessary to obtain more reliable estimates. More complex regression models, such as multi-layer perceptrons, would require a larger number of units to estimate the parameters. A possible remedy would be to consider small regions in the output as outliers. Yet within a multi-layer perceptron framework, this issue would need to be handled in the iteration process. Instead of developing separate models for each regions, a global neural network with both shared and region-specific parameters may be a promising way to integrate our framework with state-of-the-art GeoAI models, making the models aware of spatial heterogeneity by delineating corresponding regions.

We contributed to solve a puzzle of identifying regions whose models optimize both their ability to explain phenomena locally and globally. Our work provided a perspective on the current discussion on replicability, or spatial generalization of geographical models. When we derive a model from data in one place, would it be applicable to other places? We suppose that an application scope should be determined for each model, out of which different models should be used. The result would be several regional models, which can be optimized in a top-down approach with the proposed framework. One major limitation of the proposed framework is that the class of model cannot vary across regions. Future work may envisage allowing the use of different classes of models in different regions, which might find future applications.

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Data and codes availability statement

The data and codes that support the findings of this study are available on a Github repository at https://github.com/Nithouson/regreg.

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15 This is not problematic when each unit is associated with a dataset. In such cases, a model can be calibrated with data from a single unit (e.g. the gravity model introduced above).
Disclosure statement

The authors declare that they have no conflict of interest.

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References

Anselin, L., 1988. Spatial econometrics: methods and models. Dordrecht: Kluwer Academic Publishers.
Anselin, L., 2010. Thirty years of spatial econometrics. Papers in Regional Science, 89(1), 3–25.
Assunção, R.M., et al., 2006. Efficient regionalization techniques for socio-economic geographical units using minimum spanning trees. International Journal of Geographical Information Science, 20(7), 797–811.
Aydin, O., et al., 2021. A quantitative comparison of regionalization methods. International Journal of Geographical Information Science, 35(11), 2287–2315.
Bradley, J.R., Wikle, C.K., and Holan, S.H., 2017. Regionalization of multiscale spatial processes by using a criterion for spatial aggregation error. Journal of the Royal Statistical Society: Series B, 79(3), 815–832.
Brunsdon, C., Fotheringham, A.S., and Charlton, M.E., 1996. Geographically weighted regression: a method for exploring spatial nonstationarity. Geographical Analysis, 28(4), 281–298.
Clark, W.A.V., and Avery, K.L., 1976. The Effects of Data Aggregation in Statistical Analysis. Geographical Analysis, 8(4), 428–438.
Denison, D.G.T., and Holmes, C.C., 2001. Bayesian Partitioning for Estimating Disease Risk. *Biometrics*, 57(1), 143–149.

Duque, J.C., Ramos,R., and Suriñach,J., 2007. Supervised regionalization methods: A Survey. *International Regional Science Review*, 30(3), 195–220.

Duque, J.C., Church, R.L., and Middleton, R.S., 2011. The p-Regions Problem. *Geographical Analysis*, 43(1), 104-126.

Duque, J.C., Anselin, L., and Rey, S.J., 2012. The Max-p-Regions Problem. *Journal of Regional Science*, 52(3), 397–419.

Feng, X., et al., 2021. pysal/spopt[software]. Available from: https://github.com/pysal/spopt [Accessed 29 October 2021]. doi: 10.5281/zenodo.4444156.

Folch, D.C., and Spielman, S.E., 2014. Identifying regions based on flexible user-defined constraints. *International Journal of Geographical Information Science*, 28(1), 164–184.

Fotheringham, A.S., 2020. Local modeling: one size does not fit all. *Journal of Spatial Information Science*, 21, 83–87.

Fotheringham, A.S. and Brunsdon, C., 1999. Local Forms of Spatial Analysis. *Geographical Analysis*, 31(4), 340–358.

Fotheringham, A.S. and Sachdeva, M., 2022. Modelling spatial processes in quantitative human geography. *Annals of GIS*, 28(1), 5–14.

Fotheringham, A.S., and Wong, D.W.S., 1991. The modifiable areal unit problem in multivariate statistical analysis. *Environment and Planning A*, 23(7), 1025–1044.

Fotheringham, A.S., Brunsdon, C., and Charlton, M., 2002. Geographically weighted regression: the analysis of spatially varying relationships. Hoboken: John Wiley & Sons.

Fotheringham, A.S., Yang, W., and Kang, W., 2017. Multiscale Geographically Weighted Regression (MGWR). *Annals of the American Association of Geographers*, 107(6), 1247–1265.

Gelman, A., and Hill, J., 2007. Data Analysis Using Regression and Multilevel/Hierarchical Models. Cambridge: Cambridge University Press.

Getis, A., 1991. Spatial interaction and spatial autocorrelation: a cross-product approach. *Environment and Planning A*, 23, 1269–1277.

Goodchild, M.F., 2004. GIScience, Geography, Form, and Process. *Annals of the Association of American Geographers*, 94(4), 709–714.

Goodchild, M.F. and Li, W., 2021. Replication across space and time must be weak in the social and environmental sciences. *Proceedings of the National Academy of Sciences of the United States of America*, 118(35), e2015759118.

Griffith, D.A., 2008. Spatial-Filtering-Based Contributions to a Critique of Geographically Weighted Regression (GWR). *Environment and Planning A*, 40(11), 2751–2769.

Guo, D., 2008. Regionalization with dynamically constrained agglomerative clustering and partitioning (REDCAP). *International Journal of Geographical Information Science*, 22(7), 801–823.

Harris, C.R., et al, 2020. Array programming with NumPy. *Nature* 585, 357–362.

Karypis, G., Han, E.-H., and Kumar, V., 1999. Chameleon: Hierarchical Clustering Using Dynamic Modeling. *Computer*, 32(8), 68–75.

Kirkpatrick, S., Gelatt, C., Vecchi, M., 1983. Optimization by Simulated Annealing. *Science*, 220, 671–680.

Knorr-Held, L., and Raßer, G., 2000. Bayesian Detection of Clusters and Discontinuities in Disease Maps. *Biometrics*, 56(1), 13–21.

Li, F., and Sang, H., 2019. Spatial Homogeneity Pursuit of Regression Coefficients for Large Datasets. *Journal of the American Statistical Association*, 114, 1050–1062.

Li, W., Church, R.L., and Goodchild, M.F., 2014. The p-Compact-regions Problem. *Geographical Analysis*, 46(3), 250–273.

Liu, Y., et al, 2022. A note on GeoAI from the perspective of geographical laws. *Acta Geodaetica et Cartographica Sinica*, 51(6), 1062–1069.

Luo, Z.T., Sang, H., and Mallick, B., 2021. A Bayesian Contiguous Partitioning Method for Learning Clustered Latent Variables. *Journal of Machine Learning Research*, 22, 1–52.

Ma, Z., Xue, Y., and Hu, G., 2020. Heterogeneous regression models for clusters of spatial
dependent data. *Spatial Economic Analysis*, 15(4), 459–475.

MacQueen, J., 1967. Some methods for classification and analysis of multivariate observations. In: *Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability*, Volume 1: Statistics, Berkeley and Los Angeles: University of California Press, 281–296.

Openshaw, S., 1977. A geographical solution to scale and aggregation problems in region-building, partitioning and spatial modelling. *Transactions of the Institute of British Geographers*, 2(4), 459–472.

Openshaw, S., 1978. An empirical study of some zone design criteria. *Environment and Planning A*, 10(7), 781–794.

Openshaw, S. and Rao, L., 1995. Algorithms for reengineering 1991 census geography. *Environment and Planning A*, 27(3), 425–446.

Openshaw, S., and Wymer, C., 1995. Classifying and regionalizing census data. In: S. Openshaw, ed. *Census users’ handbook*. Cambridge, UK: GeoInformation International, 239–270.

Oshan, T. M., et al., 2019. MGWR: A python implementation of multiscale geographically weighted regression for investigating process spatial heterogeneity and scale. *ISPRS International Journal of Geo-Information*, 8, 269.

Pedregosa, F., et al., 2011. Scikit-learn: Machine Learning in Python. *Journal of Machine Learning Research*, 12, 2825–2830.

Rand, W.M., 1971. Objective Criteria for the Evaluation of Clustering Methods. *Journal of the American Statistical Association*, 66, 846–850.

Rey, S.J., et al., 2021. The PySAL Ecosystem: Philosophy and Implementation. *Geographical Analysis*, in press, doi: 10.1111/gean.12276.

Shaver, G.R., 2005. Spatial Heterogeneity: Past, Present, and Future. In: Lovett, G.M., et al., ed. *Ecosystem Function in Heterogeneous Landscapes*. New York, NY: Springer, 443–449.

Sui, D., Kedron, P., 2021. Reproducibility and Replicability in the Context of the Contested Identities of Geography. *Annals of the American Association of Geographers*, 111(5), 1275–1283.

Teixeira, L.V., Assunção, R.M., Loschi, R.H., 2019. Bayesian Space-Time Partitioning by Sampling and Pruning Spanning Trees. *Journal of Machine Learning Research*, 20, 1–35.

Tobler, W.R., 1970. A Computer Movie Simulating Urban Growth in the Detroit Region. *Economic Geography*, 46(2), 234–240.

Tong, D., Murray, A.T., 1970. Spatial optimization in geography. *Annals of the American Association of Geographers*, 102(6), 1290–1309.

Vinh, N.X., Epps, J., Bailey, J., 2010. Information Theoretic Measures for Clusterings Comparison: Variants, Properties, Normalization and Correction for Chance. *Journal of Machine Learning Research*, 11, 2837–2854.

Wang, J., Zhang, T., and Fu, B., 2016. A measure of spatial stratified heterogeneity. *Ecological Indicators*, 67, 250–256.

Wei, R., Rey, S., and Knaap, E., 2021. Efficient regionalization for spatially explicit neighborhood delineation. *International Journal of Geographical Information Science*, 35(1), 135–151.

Wei, R., Rey, S., and Grubesic, T.H., 2022. A Probabilistic Approach to Address Data Uncertainty in Regionalization. *Geographical Analysis*, 54, 405–426.

Xie, Y., et al., 2021. Spatial-Net: A self-adaptive and model-agnostic deep learning framework for spatially heterogeneous datasets. In: Proceedings of 29th International Conference on Advances in Geographic Information Systems (SIGSPATIAL’21), 2-5 November 2021 Beijing. New York: Association for Computing Machinery, 313–323.

Xu, L., et al., 2011. Nonlinear effect of climate on plague during the third pandemic in China. *Proceedings of the National Academy of Sciences of the United States of America*, 108(25), 10214–10219.

Yu, H., et al., 2020. Inference in Multiscale Geographically Weighted Regression. *Geographical Analysis*, 52(1), 87–106.

Zhang, Z., Li, C.Y., and Maiti, T., 2014. Analyzing 2000–2010 Childhood Age-Adjusted Cancer Rates in Florida: A Spatial Clustering Approach. *Statistics and Public Policy*, 1(1), 120–128.
Figure A1. Results on algorithm stability and running time. (a) Boxplot showing the objective function values of solutions produced by four algorithms (K-Models (blue), AZP (orange), Regional-K-Models (green), and GWR (red)). Each algorithm is executed 50 times on a simulation from Dataset 2. (b) Average running time of each algorithm to carry out the simulated experiments. Three cases on Dataset 1 are labeled 1A (low noise, \( \sigma = 0.1 \)), 1B (medium noise, \( \sigma = 0.2 \)), and 1C (high noise, \( \sigma = 0.3 \)). Two cases on Dataset 2 is labeled 2A (\( \lambda = 5 \)) and 2B (\( \lambda = 3 \)). The times reported include multiple trials for different \( K \) values (2 to 20 for K-Models, AZP, and Regional-K-Models; 2 to 60 for GWR).

Appendix A. Algorithm stability and running time

To examine the stability of the proposed zoning optimization algorithms, we take one simulation from Dataset 2, and repeat the regionalization process with each algorithm for 50 times. Figure A1a shows the distributions of objective function values. Even considering 50 repeats, no results from the spatially explicit methods, AZP and Regional-K-Models, are comparable with K-Models and GWR. Moreover, GWR and K-Models show less variability in repeating runs, indicating better stability compared to the spatially explicit methods. We infer that the merging process might have enhanced the algorithm stability. K-Models produces better solution than GWR in most cases but exhibits a slightly larger variability.

Figure A1b shows the running time of the four algorithms on simulated datasets. These algorithms took about ten minutes to half an hour to regionalize a 25 \( \times \) 25 grid. The time cost is considerably larger than attribute-based regionalization due to the larger time complexity associated with the model parameter estimation in a linear regression setting. Of the four algorithms, Regional-K-Models is the fastest and is considerably faster than AZP, as the latter considers a wider range of candidate moves. The time cost of K-Models is comparable with AZP and GWR.

Appendix B. Discussion on the parameters \( \lambda \) and \( K \)

In the proposed framework, the value of \( \lambda \) needs to be specified as input. This parameter is associated with the trade-off between the number of regions and the overall accuracy of the models. In practice, determining a suitable value of \( \lambda \) may be challenging. In some cases, we are only interested in a specific region scale (such as the region reconstruction experiment on Dataset 1 described in Section 4.1 and 4.2), and the optimal range of \( \lambda \) can be empirically identified with a relatively low number of trials. For users without any particular constraints on the region scale, we suggest
Figure B1. The estimated Pareto front for an experiment on a simulation from Dataset 2 using K-Models, with $\lambda$ varying from 1 to 20. The markers stand for Pareto optimal solutions. The results reflect the trade-off between accuracy (minimizing the overall modelling error $E$) and generality (minimizing the number of regions $\gamma$).

running the algorithms with different $\lambda$ values, which will produce a range of possible results. Here the optimization problem can be viewed as multi-objective which jointly minimizes the modelling error $E$ and the number of regions $\gamma$. For each $\gamma$, we take the solution with the lowest modelling error $E$. These solutions are called “Pareto optimal” (Tong and Murray 2012). The Pareto front is composed of all Pareto optimal solutions and reflects the trade-off between accuracy and generality. Figure B1 illustrates the estimated Pareto front from the K-Models algorithm, carried out on a simulation from Dataset 2, with $\lambda = 1, 2, \ldots, 20$. As $\lambda$ increases, the number of regions $\gamma$ decreases from 13 to 2. All the Pareto solutions represent the heterogeneity of the spatial phenomenon at different region scales.

We investigate the effects of the input parameter $K$ on Dataset 1 with a low noise (Figure B2). In this case, the true parameter distribution consists of five distinct regions. Although a series of $K$ values could be tested, the choice of $K$ is not that important in K-Models because of the merging procedure. Any choice of $K$ from 5 to 20 produces satisfying result, as the algorithm merges the $K$ initial regions into around 5 regions. The results for GWR show that the objective function decreases slowly with an increase in $K$ on average. The best solution usually corresponds to a relatively large $K$ value (between about 40 and 50). As for AZP and Regional-K-Models, the parameter $K$ determines the number of produced regions. The best choice of $K$ seems to be below 10 (4 for Regional-K-Models and 9 for AZP). As expected, the values of the objective function increases as $K$ gets larger. Considering one run only, we note a relatively high variation in the objective function values associated with $K$, which seems to affect AZP and Regional-K-Models in particular (Figure B2).
Figure B2. Effects of the parameter $K$ on the objective function value for K-Models (blue), AZP (orange), Regional-K-Models (green), and GWR (red). (a) Mean objective function values at different $K$ values from the experiment on 50 simulations in Dataset 1, with low noise ($\sigma = 0.1$). (b) Objective function values for different $K$ in one simulation in Dataset 1, with low noise.