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1 Geographically weighted regression for 2 compositional data: An application to the U.S. 3 household income compositions

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19 — Abstract —

20 This study builds a bridge between the literatures for geographically weighted regression (GWR)
21 and compositional data analysis (CoDA). GWR allows the modeling of spatial heterogeneity in
22 regression models and is increasingly used in various fields. CoDA provides unique and useful tools for
23 compositional data, which are restricted by a constant-sum constraint. Although compositional data
24 are common in many scientific areas, it is not until recently that increasingly sophisticated statistical
25 methods have been deeply investigated. Many types of spatial models based on geostatistics, spatial
26 statistics, and spatial econometrics for compositional data have been proposed. However, there is less
27 attention to both spatial heterogeneity and the constant-sum constraint. In this study, we propose
28 a GWR model for compositional data. This allows us to model spatially varying relationships
29 while considering the constant-sum constraint. We applied this model to analyze household income
30 compositions at the county level in the US. The interpretational usefulness of the results of spatially
31 varying compositional semi-elasticities is empirically performed.

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1 Introduction

Geographically weighted regression (GWR) [2] has been widely used in various fields. The extension for non-Gaussian distributed data has also been progressing. However, studies on the extension for compositional data, which are restricted by a constant-sum constraint such as 1 for proportions and 100 for percentages, are quite limited.

Although compositional data are commonly found in various scientific areas, it has not been until recently that the statistical analysis for compositional data, typically termed compositional data analysis (CoDA) [1, 5], has gained momentum. Currently, the development of spatial regression models for compositional data is one of hot topics in the CoDA literature. Geostatistical compositional models such as compositional kriging is popular approaches because CoDA are historically developed in geosciences in which a continuous spatial process can naturally be assumed. In other words, models with a discrete spatial process are relatively limited. Some papers employ conditional autoregressive models [9] or simultaneous autoregressive (spatial econometric) models [8]. In these models, spatial auto-correlation are considered. However, models for compositional data with spatial heterogeneity or spatially varying relationships are still quite limited.

The objective of this study is to propose a GWR model for compositional data to consider spatial heterogeneity and the constant-sum constraint. We accommodate the GWR model and logratio techniques of CoDA, and then formulate the GWR model in the simplex space, which is the sample space of compositional data.

2 Fundamental concepts and operators of CoDA

2.1 Aitchison geometry in the simplex space

A vector $\mathbf{p} = (p_1, p_2, \dots, p_D)$ whose components are positive real numbers and carry relative information is called as a D -part composition. The composition can be represented as an element of the D -part simplex space \mathcal{S}^D :

$$\mathcal{S}^D = \left\{ \mathbf{p} = (p_1, p_2, \dots, p_D) \mid p_m > 0, m = 1, 2, \dots, D, \sum_{m=1}^D p_m = \kappa \right\}, \quad (1)$$

where κ is a constant sum for compositions in \mathcal{S}^D . Usual values of κ are 1 (proportions) and 100 (percentages: %). Rescaling of compositions can be formalized by the closure

$$\text{operator } \mathcal{C}_\kappa \text{ for } \mathbf{z} = (z_1, z_2, \dots, z_D) \in \mathbb{R}_+^D: \mathcal{C}_\kappa(\mathbf{z}) = \left(\frac{\kappa \cdot z_1}{\sum_{m=1}^D z_m}, \frac{\kappa \cdot z_2}{\sum_{m=1}^D z_m}, \dots, \frac{\kappa \cdot z_D}{\sum_{m=1}^D z_m} \right).$$

The constant-sum constraint induces statistical problems such as the restriction of the degree of freedom and the spurious correlation for the use of standard statistical methods with compositions [1].

The geometrical structure of compositions has been established to define a vector space structure of the simplex space, and it is referred as the Aitchison geometry. The two basic operations are the perturbation operator and the powering operator which correspond to the addition/shifting operator and the multiplication operator in the Euclidean geometry, respectively. For two D -part compositions $\mathbf{p}, \mathbf{q} \in \mathcal{S}^D$ and a constant scalar $\alpha \in \mathbb{R}$, the perturbation operator \oplus is: $\mathbf{p} \oplus \mathbf{q} = \mathcal{C}_\kappa(p_1 \cdot q_1, p_2 \cdot q_2, \dots, p_D \cdot q_D) \in \mathcal{S}^D$ and the power operator \odot is: $\alpha \odot \mathbf{p} = \mathcal{C}_\kappa(p_1^\alpha, p_2^\alpha, \dots, p_D^\alpha) \in \mathcal{S}^D$. By using the two fundamental operators, for $\mathbf{p}_k \in \mathcal{S}^D$, $\alpha_k \in \mathbb{R}$, $k = 1, 2, \dots, K$, the perturbation-linear combination operator \bigoplus is introduced: $\bigoplus_{k=1}^K \alpha_k \odot \mathbf{p}_k = \alpha_1 \odot \mathbf{p}_1 \oplus \alpha_2 \odot \mathbf{p}_2 \oplus \dots \oplus \alpha_K \odot \mathbf{p}_K = \mathcal{C}_\kappa \left(\prod_{k=1}^K p_{k,1}^{\alpha_k}, \prod_{k=1}^K p_{k,2}^{\alpha_k}, \dots, \prod_{k=1}^K p_{k,D}^{\alpha_k} \right) \in \mathcal{S}^D$.

81 2.2 Logratio transformation

82 Since most standard statistical methods depend on the Euclidean geometry in the real space,
 83 it is reasonable to project compositions from the simplex to the real space. To construct
 84 such projections, some transformations have been proposed. Classical transformations are
 85 the additive logratio (alr) [1]; the centered logratio (clr) [1]; and the isometric logratio
 86 (ilr) [6]. It can be said that the CoDA literature has been discussing and providing the
 87 general framework of the logratio transformation. In this paper, the ilr transformation is
 88 used because it is based on an orthonormal basis, so that it is well recognized as the most
 89 preferable from a mathematical point of view. There are infinitely many possibilities to define
 90 such an orthonormal basis. In the CoDA literature, the following ilr orthonormal coordinates
 91 referred to as the pivot coordinates [7] is currently used as a preferable option. The ilr
 92 transformation with the pivot coordinates for $\mathbf{p} \in \mathcal{S}^D$ is defined as follows: $\text{ilr}(\mathbf{p}) = \mathbf{p}^* =$
 93 $(p_1^*, p_2^*, \dots, p_{D-1}^*) \in \mathbb{R}^{D-1}$ with $p_l^* = \sqrt{\frac{D-j}{D-j+1}} \ln \frac{p_j}{\sqrt[{}^{D-j}]{\prod_{\tilde{m}=1}^D p_{\tilde{m}}}}, l = 1, 2, \dots, (D-1)$, where
 94 superscript * denotes the ilr transformation.

95 3 GWR model for compositional data

96 The GWR model is an extension of the linear regression model that allows regression
 97 coefficients to vary across geographical space. When the explained variable is a D -part
 98 composition, the basic GWR model in the simplex \mathcal{S}^D can be expressed as follows:

$$99 \quad \mathbf{y}_i = \bigoplus_{k=1}^{K+1} (x_{i,k} \odot (\boldsymbol{\beta}_i)_k) \oplus \boldsymbol{\varepsilon}_i, \quad (2)$$

100 where $i \in \{1, 2, \dots, n\}$ is the index for sites; \mathbf{y}_i is the explained variables; $x_{i,k}$ is the k -th
 101 covariate; $K+1$ is the number of covariates including intercept; $(\boldsymbol{\beta}_i)_k$ is unknown parameters
 102 of $x_{i,k}$; $\boldsymbol{\varepsilon}_i$ is the disturbances. \mathbf{y}_i , $(\boldsymbol{\beta}_i)_k$, and $\boldsymbol{\varepsilon}_i$ are D -part compositions in \mathcal{S}^D . In order
 103 to estimate parameters of the model, we consider the following two characteristics: (1)
 104 constant-sum constraint and (2) spatial heterogeneity.

105 STEP 1: For considering the constant-sum constraint of compositional explained variables
 106 and obtaining the model in real space, we use the ilr transformation. The ilr transformed
 107 model for the i -th observation site in the l -th GWR model as a scalar representation can be
 108 expressed as $y_i^{*(l)} = \sum_{k=1}^{K+1} \left(x_{i,k} \cdot \left(\boldsymbol{\beta}_i^{*(l)} \right)_k \right) + \varepsilon_i^{*(l)}$.

109 STEP 2: Each transformed model can be estimated independently [4]. Therefore, the
 110 estimation of the basic GWR model can be applied. Thus, the regression coefficients $\boldsymbol{\beta}_i^{*(l)}$ is
 111 given by the weighted least squares estimators as: $\hat{\boldsymbol{\beta}}_i^{*(l)} = [\mathbf{X}' \mathbf{G}_i(b^{(l)}) \mathbf{X}]^{-1} \mathbf{X}' \mathbf{G}_i(b^{(l)}) \mathbf{y}^{*(l)}$,
 112 where \mathbf{X} is the covariates matrix whose (i, k) -th element equals $x_{i,k}$, $\mathbf{G}_i(b^{(l)})$ is an $n \times n$
 113 diagonal matrix, whose j -th element assigns the weight on the j -th sample site. The weight
 114 is given by a distance-decaying kernel, which we assumed the Gaussian kernel. $b^{(l)}$ is the
 115 kernel bandwidth, which can vary for each l . The GWR model can be estimated by first
 116 optimizing the bandwidth, and estimating the regression coefficients $\boldsymbol{\beta}_i^{*(l)}$ after that. The
 117 bandwidth can be optimized by the leave-one-out cross-validation method to minimize the
 118 cross-validation score.

119 **4 Empirical analysis**

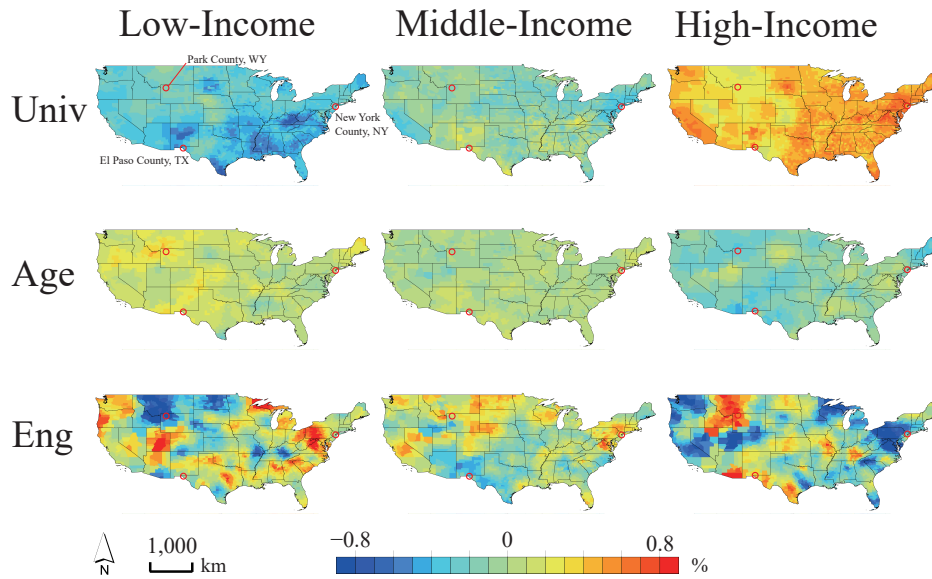
120 **4.1 Outline**

121 This section illustrates an application of our proposed model to the United States (US) house-
 122 hold income dataset 2017. The explained variable is county-level compositional household
 123 income data divided into the high-income bracket with households whose income in the past
 124 12 months was more than \$75,000, middle-income bracket with households earning between
 125 \$35,000–\$75,000, and low-income bracket of less than \$35,000. The sample size is 3,108. To
 126 maintain a continuous geographical space, Alaska and Hawaii are excluded from the sample.
 127 To discuss regional differences, we selected three counties: New York County, New York
 128 (NY), El Paso County, Texas (TX), and Park County, Wyoming (WY). The covariates are as
 129 follows: *Univ* is the percentage of people with a bachelor’s degree or higher among people
 130 over 25 years old, *Eng* is the percentage of people who speak English, and *Age* is the median
 131 age.

132 **4.2 Results**

133 Figure 1 summarizes the estimated semi-elasticities of each covariate for each bracket. Because
 134 the dependent variable is transformed, it is not appropriate to directly interpret and visualize
 135 the regression coefficients. The semi-elasticity gives the relative percentage change in the
 136 dependent variable when the covariate increases by 1 unit. It is noted that the sum of the
 137 semi-elasticities for each bracket in the compositional model is 0. This helps us easily and
 138 directly interpret the impact. Additionally, thanks to the GWR model, the semi-elasticity
 139 spatially varies. For example, when the covariate *Univ* of New York County increases by 1
 140 unit, high income changes +0.513%, middle income –0.256%, and low income –0.257%. In
 141 the same way, for El Paso County, high income changes +0.509%, middle income –0.006%,
 142 and low income –0.443%. For Park County, high income changes +0.282%, middle income
 143 –0.151%, and low income –0.131%. As a result, the impact on the low-income households of
 144 New York County is about two times that of Park County. From the spatial distributions in
 145 Figure 1, *Univ* has a positive impact on the high-income bracket, especially in metropolitan
 146 counties on the east and west coasts. Because there are many white-collar and professional
 147 workers living in these counties, this result is reasonable. *Age* has a positive impact on the
 148 low-income bracket. *Age* also has a positive impact on the high-income bracket of some
 149 counties in the eastern area. Based on the results, older veteran workers have higher earnings
 150 in these counties. *Eng* has a strong impact on each bracket. In the northwestern area, *Eng*
 151 has a strong positive impact on the high-income bracket and a strong negative impact on the
 152 low-income bracket. In the southern area, which is close to the Mexico-US border, speaking
 153 English appears to have a positive impact on the high-income bracket.

154 Figure 2 illustrates the effects of the inverse-transformed estimated coefficients, in which
 155 the change in the predicted probabilities for each bracket can be seen as a function of the
 156 change in the covariate level. When we hold the non-target covariates at the observed
 157 values, we can examine the predicted probabilities across the observed range of each covariate
 158 individually. In the model, the predicted probabilities are also spatially varying, so the results
 159 can be comparable among sites. From the comparison of the three counties, *Univ* shows a
 160 positive impact regarding high-income households, with the strongest relationship occurring
 161 in New York County. When *Univ* is around 8% – 10%, the most dominant bracket changes.
 162 Among the three counties, *Age* and *Eng* exhibit different patterns. In New York County, *Age*
 163 does not affect much change. *Age* has a linearly increasing effect on the low-income bracket



■ **Figure 1** Semi-elasticity of each covariate for each bracket.

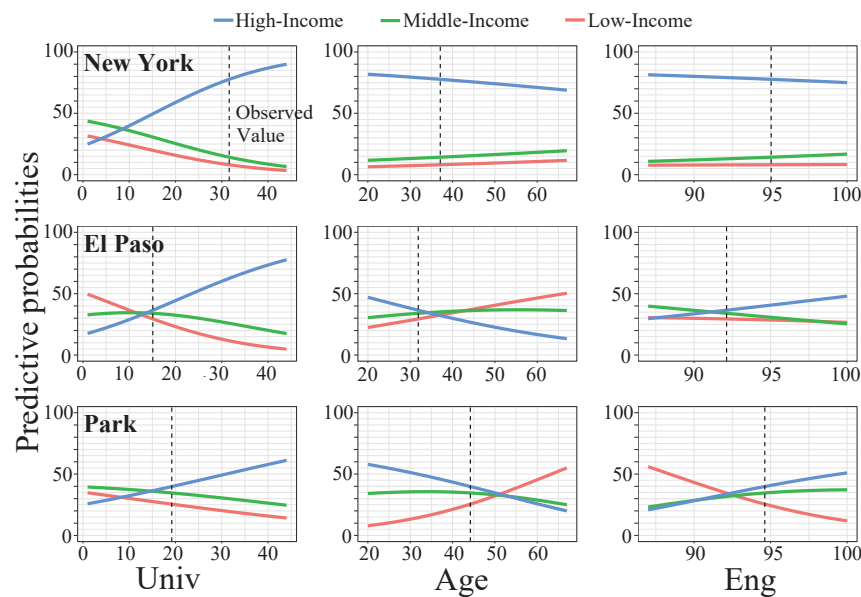
164 in El Paso and an exponential effect in Park. Although *Eng* in New York does not change
 165 the income brackets much, the high-income brackets increase in El Paso and Park. In Park,
 166 *Eng* exponentially decreases the low-income bracket.

167 In summary, the study provides an empirical evidence that our proposed model successfully
 168 captures spatial patterns in the regression results. Although the regression coefficients
 169 cannot be interpreted, the semi-elasticities and predicted probabilities are directly and easily
 170 interpretable. The model can be useful for a wide variety of spatial modeling with spatial
 171 heterogeneity and compositional characteristics.

172 **5 Discussion and conclusion**

173 This study aims to develop a methodology for geographically weighted regression (GWR) for
 174 compositional data that models spatially varying coefficients restricted in a simplex space.
 175 These findings are meaningful because spatial compositional data are common in many
 176 fields, including environmental sciences and geography. An analysis of household income
 177 compositional data in the United States demonstrated that spatially varying compositional
 178 semi-elasticities with a sum restricted to 0 and spatially varying predicted probabilities
 179 provide insights into a spatial non-stationary phenomenon.

180 Our proposed model can be considered in the extension of GWR modeling for non-
 181 Gaussian distributed data, which has been progressing in the spatial analysis literature. [3]
 182 proposes a geographically weighted beta regression for a rate or proportion that is usually
 183 defined between (0, 1). Naturally, one potential extension is to consider Dirichlet distributed
 184 data. Developing a geographically weighted Dirichlet regression and comparing it with our
 185 approach is an interesting topic for future research.



■ **Figure 2** Predictive probabilities for each bracket regarding each covariate for New York County, NY (top), El Paso County, TX (middle), and Park County, WY (bottom). In each panel, the target covariate varies across the observed range of data and the non-target covariates are held at the observed values.

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