Local variable selection and parameter estimation for spatially varying coefficient models

Wesley Brooks

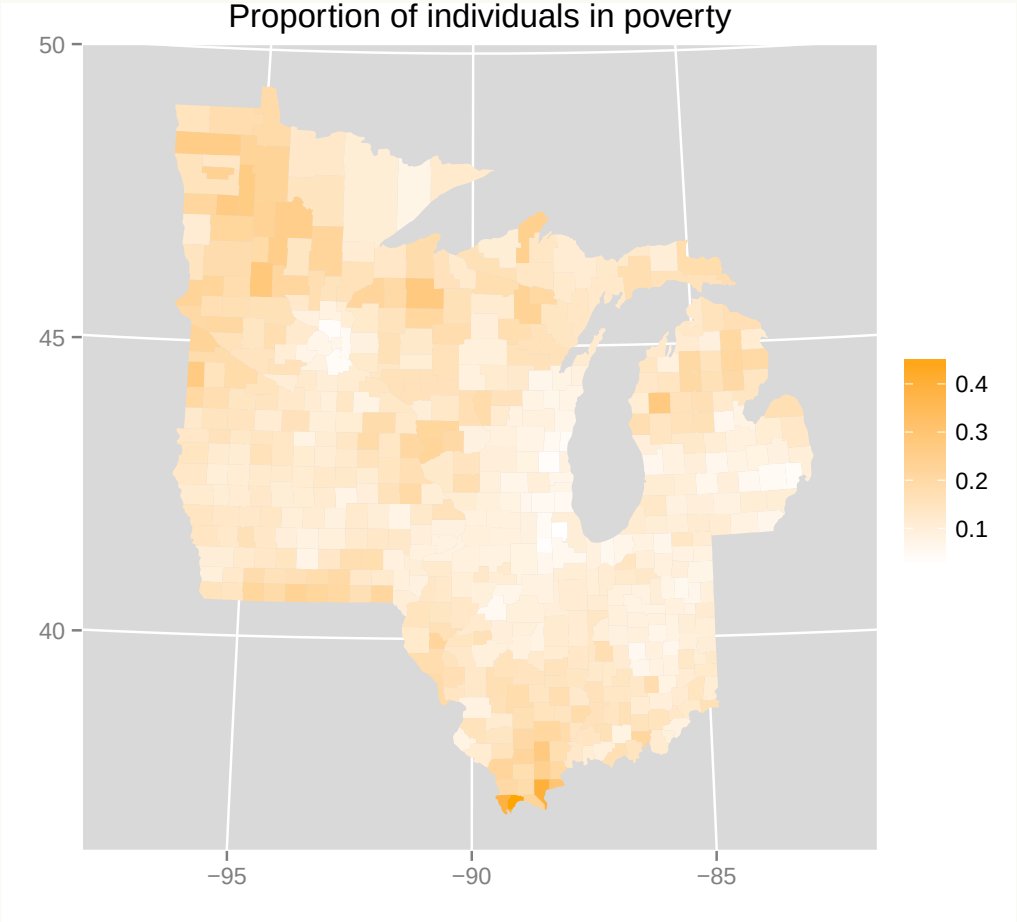
Department of Statistics
University of Wisconsin–Madison

November 1, 2013

Motivation

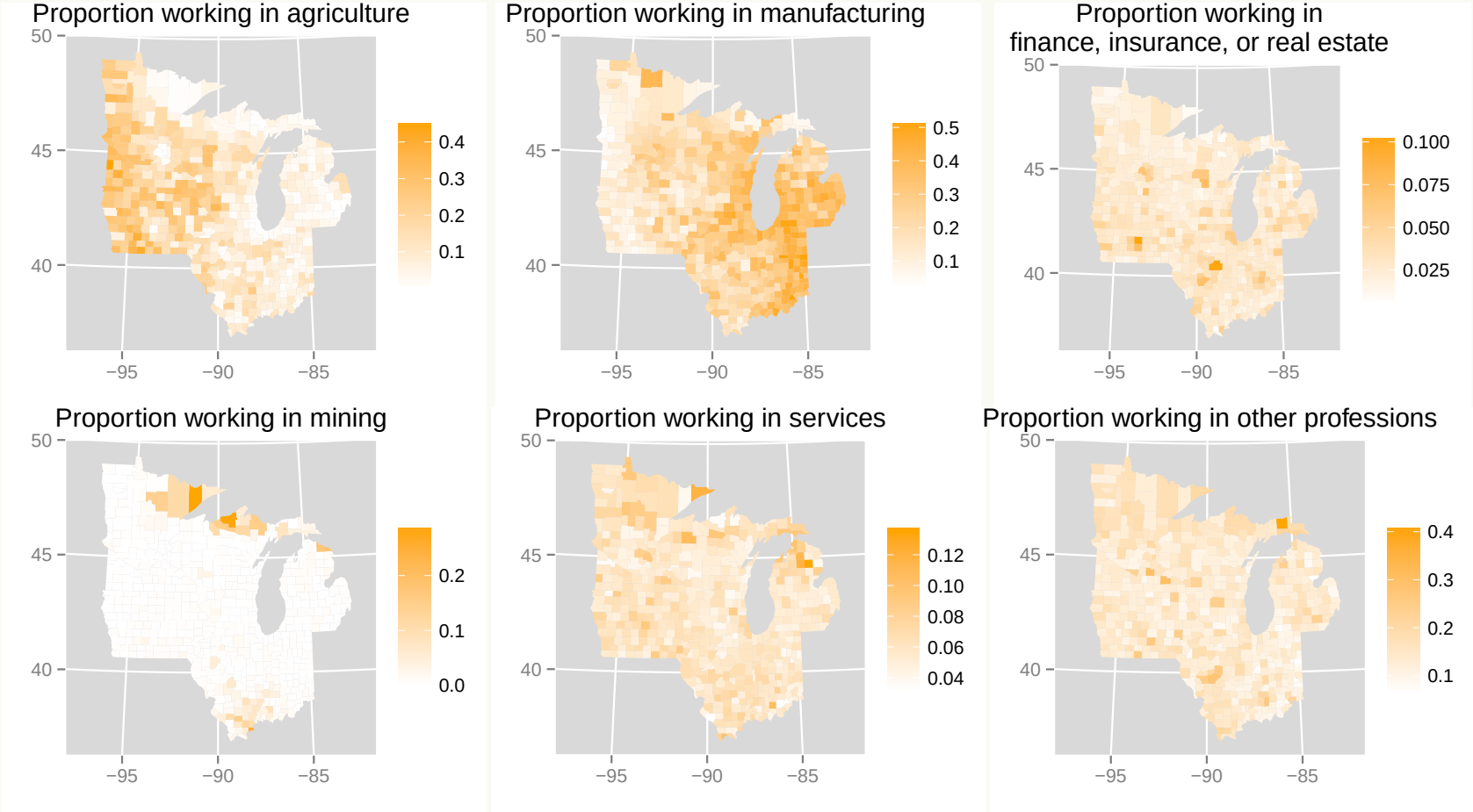
Motivation

Take a look at some data



Motivation

Take a look at some data



Motivation

Sensible questions about the data

- Which of the economic-structure variables is associated with poverty rate?
- What are the sign and magnitude of that association?
- Is poverty rate associated with the same economic-structure variables across the entire region?
- Are the sign and magnitude of the associations constant across the region?

Introduction

Introduction

A review of existing methods

- Spatial regression
- Varying coefficient regression
  - Splines
  - Kernels
  - Wavelets
- Model selection via regularization

Introduction

Some definitions

- Univariate spatial response process $\{Y(\boldsymbol{s}) : \boldsymbol{s} \in \mathcal{D}\}$
- Multivariate spatial covariate process $\{\boldsymbol{X}(\boldsymbol{s}) : \boldsymbol{s} \in \mathcal{D}\}$
- $n =$ number of observations
- $p =$ number of covariates
- Location (2-dimensional) $\boldsymbol{s}$
- Spatial domain $\mathcal{D}$

Introduction

Further definitions

- Geostatistical data:
  - Observations are made at sampling locations $\boldsymbol{s}_i$ for $i = 1, \ldots, n$
  - E.g. elevation, temperature
- Areal data:
  - Domain is partitioned into n regions $\{D_1, \ldots, D_n\}$
  - The regions do not overlap, and they divide the domain completely: $\mathcal{D} = \bigcup_{i=1}^{n} D_i$
  - Sampling locations $\boldsymbol{s}_i$ for $i = 1, \ldots, n$ are the centroids of the regions
  - E.g. poverty rate, population, spatial mean temperature

Introduction

Spatial regression (Cressie, 1993)

- The typical spatial regression

$$
\begin{aligned}
Y(\boldsymbol{s}) &= \boldsymbol{X}(\boldsymbol{s})'\boldsymbol{\beta} + W(\boldsymbol{s}) + \varepsilon(\boldsymbol{s}) \\
\text{cov}(W(\boldsymbol{s}), W(\boldsymbol{t})) &= \Gamma\left(\delta(\boldsymbol{s}, \boldsymbol{t})\right) \\
\delta(\boldsymbol{s}, \boldsymbol{t}) &= \sqrt{\|\boldsymbol{t} - \boldsymbol{s}\|_2} \\
\text{E.g. } \Gamma(\delta(\boldsymbol{s}, \boldsymbol{t})) &= \exp\{-\phi^{-1}\delta(\boldsymbol{s}, \boldsymbol{t})\} \qquad (1)
\end{aligned}
$$

- $W(\boldsymbol{s})$ is a spatial random effect that accounts for autocorrelation in the response variable
- The coefficients $\boldsymbol{\beta}$ are constant
- Relies on *a priori* global variable selection

Introduction

Spatially varying coefficient process (Gelfand et al., 2003)

- Making model more flexible: coefficients in a spatial regression model can be allowed to vary

$$Y(\boldsymbol{s}) = \boldsymbol{X}(\boldsymbol{s})'\boldsymbol{\beta}(\boldsymbol{s}) + \varepsilon(\boldsymbol{s})$$

- The spatial random effect has been incorporated into the spatially varying intercept
- $\{\beta_1(\boldsymbol{s}) : \boldsymbol{s} \in \mathcal{D}\}, \ldots, \{\beta_p(\boldsymbol{s}) : \boldsymbol{s} \in \mathcal{D}\}$ are stationary spatial processes with Matèrn covariance functions
- Still relies on *a priori* global variable selection

Introduction

Varying coefficients regression (Hastie and Tibshirani, 1993)

$$Y(\boldsymbol{s}) = \boldsymbol{X}(\boldsymbol{s})'\boldsymbol{\beta}(\boldsymbol{s}) + \varepsilon(\boldsymbol{s})$$

- Assume an effect modifying variable S
- Coefficients are functions of S

Introduction

Spline-based VCR models (Wood, 2006)

- Splines are a way to parameterize smooth functions
- Splines can be incorporated into a generalized additive model (GAM):
  - $E\{Y(t)\} = f\{X_1(t)\} + \cdots + f\{X_p(t)\}$
- It is possible to parameterize a VCR model with splines for the coefficient functions:
  - $E\{Y(t)\} = \beta_1(t)X_1(t) + \cdots + \beta_p(t)X_p(t)$

Introduction

Global selection in spline-based VCR models (L. Wang, Li, and Huang, 2008; Antoniadas, Gijbels, and Verhasselt, 2012)

Regularization methods for global variable selection in VCR models:

- The integral of a function squared (e.g. $\int \{f(t)\}^2 dt$) is zero if and only if the function is zero everywhere.
- Use regularization to encourage coefficient functions to be zero
  - SCAD penalty
  - Non-negative garrote penalty

Introduction

Wavelet methods for VCR models (Shang, 2011; J. Zhang and Clayton, 2011)

- Wavelet methods: decompose coefficient function into local frequency components
- Selection of nonzero local frequency components with nonzero coefficients:
  - Bayesian variable selection
  - Lasso
- Sparsity in the local frequency components; not in the local covariates

Geographically weighted regression

Geographically weighted regression

(Brundson, S. Fotheringham, and Martin Charlton, 1998;
A. Fotheringham, Brunsdon, and M. Charlton, 2002)

- Consider observations at sampling locations $\boldsymbol{s}_1, \ldots, \boldsymbol{s}_n$
- $y(\boldsymbol{s}_i) = y_i$ the univariate response at location $\boldsymbol{s}_i$
- $\boldsymbol{x}(\boldsymbol{s}_i) = \boldsymbol{x}_i$ the $(p+1)$-variate vector of covariates at location $\boldsymbol{s}_i$
- Assume $y_i = \boldsymbol{x}_i' \boldsymbol{\beta}_i + \varepsilon_i$ where $\varepsilon \overset{iid}{\sim} \mathcal{N}(0, \sigma^2)$

Geographically weighted regression

(Brundson, S. Fotheringham, and Martin Charlton, 1998;
A. Fotheringham, Brunsdon, and M. Charlton, 2002)

- The total log likelihood is
  $\ell(\boldsymbol{\beta}) = -(1/2)\left\{n \log(2\pi\sigma^2) + \sigma^{-2}\sum_{i=1}^{n}(y_i - \boldsymbol{x}_i'\boldsymbol{\beta}_i)^2\right\}$
- With n observations and $n(p+1)$ free parameters, the model is not identifiable.
- Estimate parameters by borrowing strength from nearby observations

Geographically weighted regression

Local regression (Loader, 1999)

Local regression uses a kernel function at each sampling location to weight observations based on their distance from the sampling location.

$$L_i = \prod_{i'=1}^{n} \left(L_{i'}\right)^{w_{ii'}}$$

$$\ell_i = \sum_{i'=1}^{n} w_{ii'} \left\{ \log \sigma_i^2 + \sigma_i^{-2} \left(y_{i'} - \boldsymbol{x}_{i'}' \boldsymbol{\beta}_i\right)^2 \right\}$$

Given the weights, a local model is fit at each sampling location using the local likelihood

Geographically weighted regression

Local likelihood(Loader, 1999)

Weights are calculated via a kernel, e.g. the bisquare kernel:

$$w_{ii'} = \begin{cases} \left[1 - \left(\phi^{-1}\delta_{ii'}\right)^2\right]^2 & \text{if } \delta_{ii'} < \phi, \\ 0 & \text{if } \delta_{ii'} \geq \phi. \end{cases} \tag{2}$$

Where

- ϕ is a bandwidth parameter
- $\delta_{ii'} = \delta(\boldsymbol{s}_i, \boldsymbol{s}_{i'}) = \left\|\boldsymbol{s}_i - \boldsymbol{s}_{i'}\right\|_2$ is the Euclidean distance

Geographically weighted regression

Bandwidth estimation via the AIC_c (Hurvich, Simonoff, and Tsai, 1998)

- Smaller bandwidth: less bias, more flexible coefficient surface
- Large bandwidth: less variance, less flexible coefficient surface
- Estimate the degrees of freedom used in estmating the coefficient surface:
  - $\hat{\boldsymbol{y}} = H\boldsymbol{y}$
  - $\nu = \text{tr}(H)$
- Then the corrected AIC for bandwidth selection is: $\text{AIC}_c = 2n \log \sigma + n \left\{ \frac{n+\nu}{n-2-\nu} \right\}$

Local variable selection and parameter estimation

Geographically weighted regression

Geographically weighted Lasso (Wheeler, 2009)

Within a GWR model, using the Lasso for local variable selection is called the geographically weighted Lasso (GWL).

- The GWL requires estimating a Lasso tuning parameter for each local model
- Wheeler, 2009 estimates the local Lasso tuning parameter at location $\boldsymbol{s}_i$ by minimizing a jacknife criterion: $|y_i - \hat{y}_i|$
- The jacknife criterion can only be calculated where data are observed, making it impossible to use the GWL to impute missing data or to estimate the value of the coefficient surface at new locations
- Also, the Lasso is known to be biased in variable selection and suboptimal for coefficient estimation

Local variable selection and parameter estimation

Geographically weighted adaptive Lasso (GWAL)

- Local variable selection in a GWR model using the adaptive Lasso (AL) (Zou, 2006)
- Under suitable conditions, the AL has an oracle property for selection

$$
\begin{aligned}
\mathcal{S}(\boldsymbol{\beta}_i) &= -2\ell_i(\boldsymbol{\beta}_i) + \mathcal{J}_2(\boldsymbol{\beta}_i) \\
&= \sum_{i'=1}^{n} w_{ii'} \left\{ \log \sigma_i^2 + \left(\sigma_i^2\right)^{-1} \left(y_{i'} - \boldsymbol{x}_{i'}' \boldsymbol{\beta}_i\right)^2 \right\} \\
&\quad + \lambda_i \sum_{j=1}^{p} |\beta_{ij}| / \gamma_{ij}
\end{aligned}
$$

Local variable selection and parameter estimation

Geographically weighted adaptive elastic net (GWEN)

- Local variable selection in a GWR model using the adaptive elastic net (AEN) (Zou and H. Zhang, 2009)
- Under suitable conditions, the AEN has an oracle property for selection

$$
\begin{aligned}
\mathcal{S}(\boldsymbol{\beta}_i) &= -2\ell_i(\boldsymbol{\beta}_i) + \mathcal{J}_2(\boldsymbol{\beta}_i) \\
&= \sum_{i'=1}^{n} w_{ii'} \left\{ \log \sigma_i^2 + \left(\sigma_i^2\right)^{-1} \left(y_{i'} - \boldsymbol{x}_{i'}' \boldsymbol{\beta}_i\right)^2 \right\} \\
&+ \alpha_i \lambda_i \sum_{j=1}^{p} |\beta_{ij}| / \gamma_{ij} \\
&+ (1 - \alpha_i) \lambda_i^* \sum_{j=1}^{p} \left(\beta_{ij} / \gamma_{ij}\right)^2
\end{aligned}
$$

Local variable selection and parameter estimation

Geographically weighted adaptive elastic net (GWEN)

where $\sum_{i'=1}^{n} w_{ii'} \left(y_{i'} - \boldsymbol{x}'_{i'}\boldsymbol{\beta}_i\right)^2$ is the weighted sum of squares minimized by traditional GWR, and $\mathcal{J}_2(\boldsymbol{\beta}_i) = \alpha_i \lambda_i^* \sum_{j=1}^{p} |\beta_{ij}|/\gamma_{ij} + (1-\alpha_i)\lambda_i^* \sum_{j=1}^{p} \left(\beta_{ij}/\gamma_{ij}\right)^2$ is the AEN penalty.

Local variable selection and parameter estimation

Tuning parameter estimation

It is necessary to estimate an AL (or AEN) tuning parameter for each local model. Using the local BIC allows fitting a local model at any location within the domain

$$
\begin{aligned}
\mathsf{BIC}_i &= -2 \sum_{i'=1}^{n} \ell_{ii'} + \log \left(\sum_{i'=1}^{n} w_{ii'} \right) \mathsf{df}_i \\
&= -2 \sum_{i'=1}^{n} \log \left[\left(2\pi \hat{\sigma}_i^2 \right)^{-1/2} \exp \left\{ -\frac{1}{2} \hat{\sigma}_i^{-2} \left(y_{i'} - \boldsymbol{x}_{i'}' \hat{\boldsymbol{\beta}}_{i'} \right)^2 \right\} \right]^{w_{ii'}} \\
&\quad + \log \left(\sum_{i'=1}^{n} w_{ii'} \right) \mathsf{df}_i
\end{aligned}
\tag{3}
$$

Local variable selection and parameter estimation

Geographically weighted elastic net (GWEN)

$$= \sum_{i'=1}^{n} w_{ii'} \left\{ \log(2\pi) + \log \hat{\sigma}_i^2 + \hat{\sigma}_i^{-2} \left(y_{i'} - \boldsymbol{x}'_{i'} \hat{\boldsymbol{\beta}}_{i'} \right)^2 \right\}$$

$$+ \log \left(\sum_{i'=1}^{n} w_{ii'} \right) \mathrm{df}_i$$

Local variable selection and parameter estimation

Locally linear coefficient estimation

The GWEN and the GWAL each estimate the local coefficients for the variables that are selected for inclusion in the local model. Both the GWEN and the GWAL estimate coefficients as locally constant, as in the class of Nadaraya-Watson kernel smoothers (Härdle, 1990). As such, they suffer from the problem of biased estimation that is common to that class of models, particularly where there is a gradient to the coefficient surface at the boundary of the domain (Hastie and Loader, 1993).

In the context of nonparametric regression, the boundary-effect bias is addressed by local polynomial modeling, usually in the form of a locally linear model (Fan and Gijbels, 1996). Locally linear coefficient estimation was proposed for the traditional GWR to counter the boundary effect by N. Wang, Mei, and Yan, 2008.

Simulation study

Simulation study

Simulating covariates

Five covariates $\tilde{X}_1, \ldots, \tilde{X}_5$ were simulated by Gaussian random fields on the domain $[0,1] \times [0,1]$ on a 30×30 grid of sampling locations:

$$\tilde{X}_j \sim N(0, \Sigma) \text{ for } j = 1, \ldots, 5$$
$$\{\Sigma\}_{i,i'} = \exp\{-\tau^{-1}\delta_{ii'}\} \text{ for } i, i' = 1, \ldots, n$$

Where the covariates were simulated with colinearity, the colinearity was induced by multiplying the design matrix by the square root of the colinearity matrix:

$$\begin{aligned} \text{diag}(\Omega_{5\times5}) &= 1 \\ \text{off-diag}(\Omega_{5\times5}) &= \rho \\ X &= \tilde{X}R \end{aligned} \tag{8}$$

Where $\Omega_{5\times5} = R'R$ is the Cholesky decomposition.

Simulation study

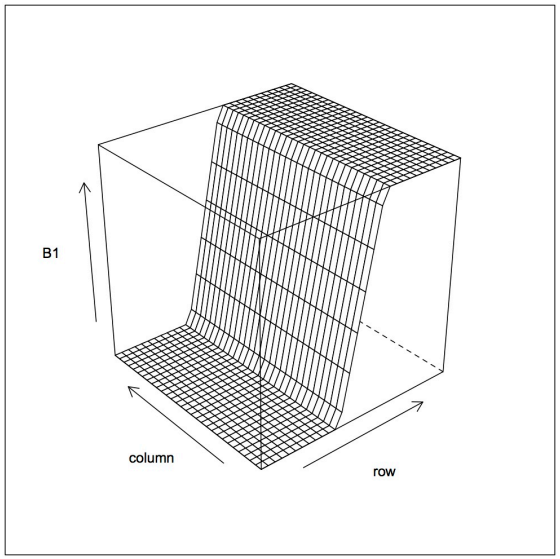
Simulating the response

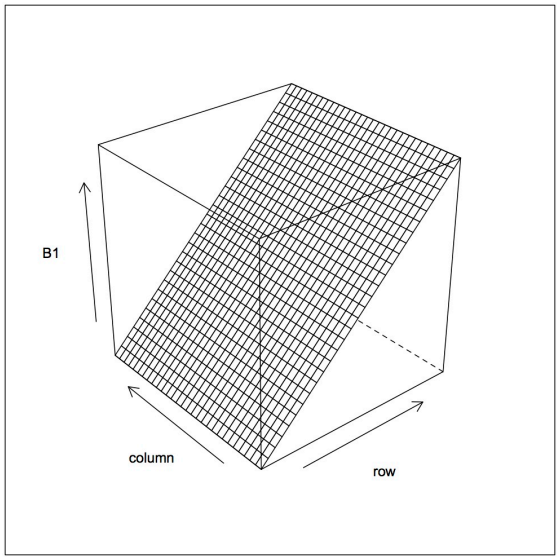
- $Y(\boldsymbol{s}) = X(\boldsymbol{s})'\boldsymbol{\beta}(\boldsymbol{s}) = \sum_{j=1}^{5} \beta_j(\boldsymbol{s}) X_j(\boldsymbol{s}) + \varepsilon(\boldsymbol{s})$
- $\boldsymbol{\varepsilon} \sim \ iid \ \ N(0, \sigma^2)$
- $\beta_1(\boldsymbol{s})$, the coefficient function for X_1, is nonzero in part of the domain.
- Coefficients for $X_2, \ldots, X_5$ are zero everywhere

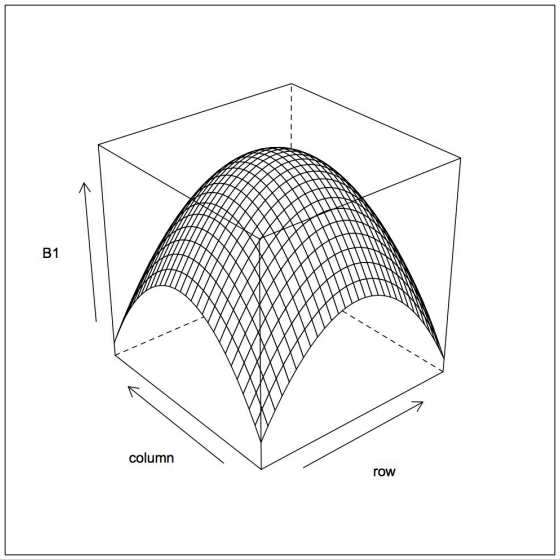
Simulation study

Coefficient functions

Call these functions step, gradient, and parabola:







Simulation study

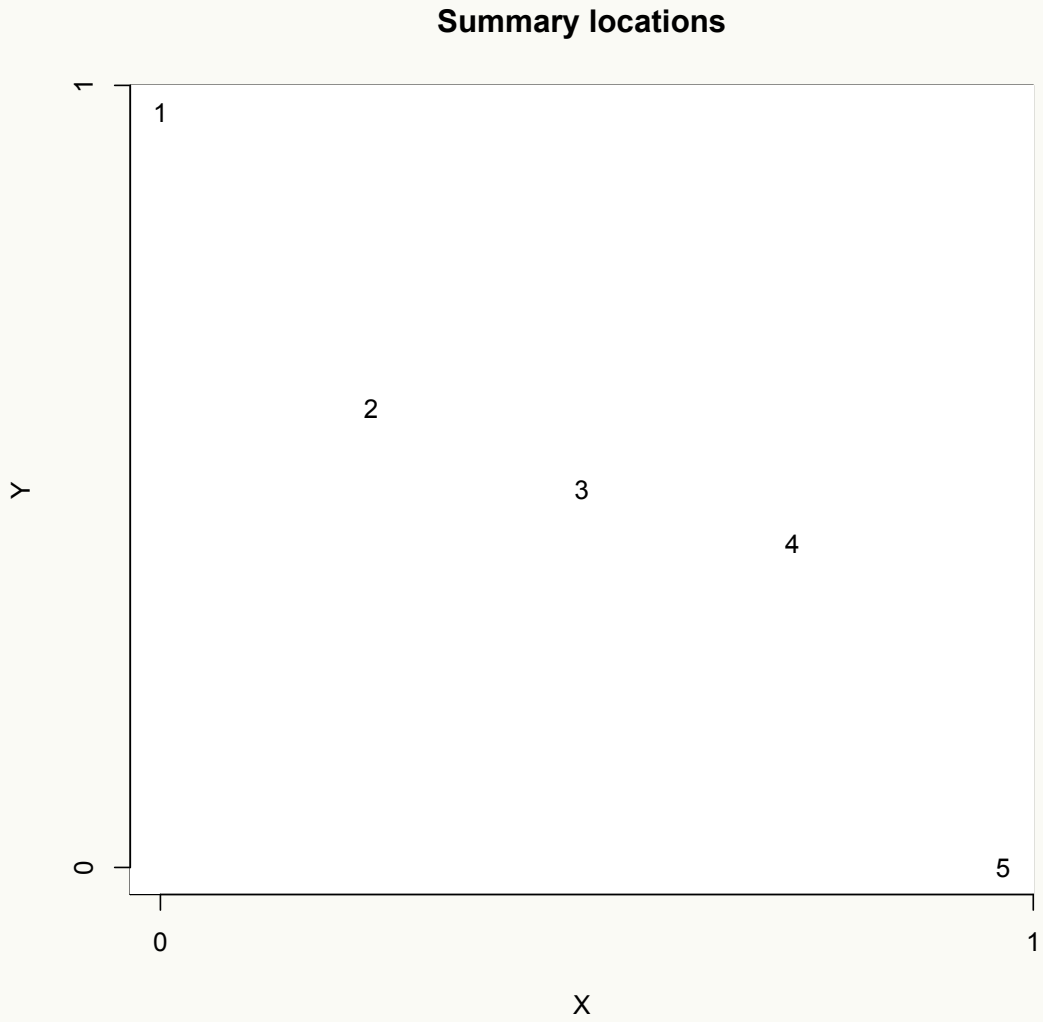
Simulation settings

Setting	function	ρ	σ^2
1	step	0	0.25
2	step	0	1
3	step	0.5	0.25
4	step	0.5	1
5	gradient	0	0.25
6	gradient	0	1
7	gradient	0.5	0.25
8	gradient	0.5	1
9	parabola	0	0.25
10	parabola	0	1
11	parabola	0.5	0.25
12	parabola	0.5	1

Table : Simulation parameters for each setting.

Simulation results

Selection



Simulation results

- 52 saw no false negatives
- 72 had no false positives
- 26 neither false positives nor false negatives

  Table **??** lists the results of variable selection. The correct covariate was usually included in the local models, and the unimportant covariates were usually excluded. Ignore for now the ambiguous locations where the true β_1 surface transitions from zero to nonzero. Of the eighty simulated cases where $\beta_1(\boldsymbol{s})$ is unambiguously nonzero, more than half (52) saw no false negatives (over 100 simulations). The number with no false negatives and no false positives (i.e. exactly the correct model was recovered in all 100 simulations) was 26. Of the 120 total simulated cases, 72 had no false positives (i.e. no variable whose true coefficient is zero was included in the model during any of the 100 simulation runs).

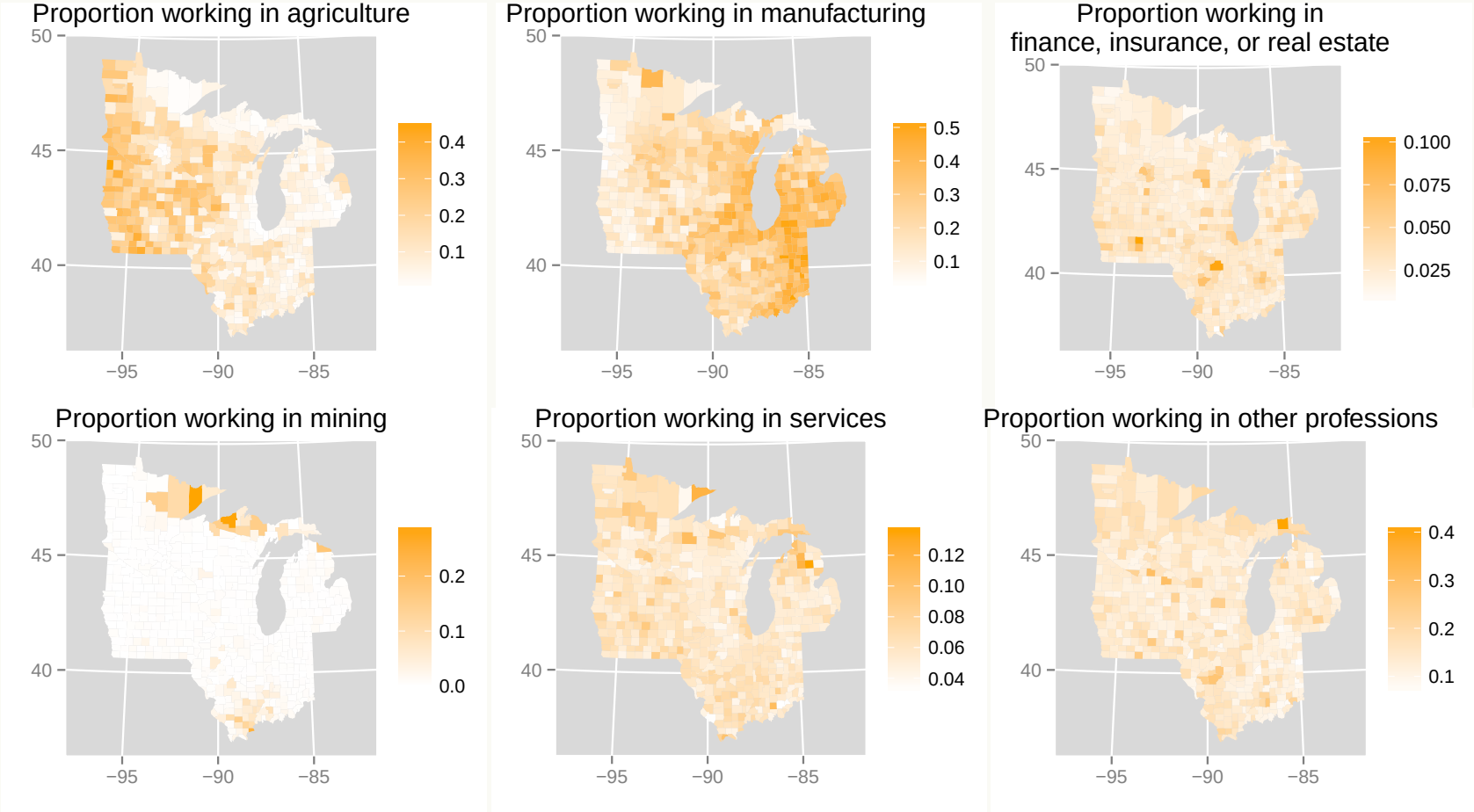
Simulation results

- The mean squared error, bias, and variance of $\hat{\beta}_1$ (MSE(β_1), bias($\hat{\beta}_1$), var($\hat{\beta}_1$)) are listed in Tables **??**, **??**, and **??**, respectively. The method of oracular selection led to the best MSE($\hat{\beta}_1$) in 41 of the 60 cases.
  In terms of MSE($\hat{\beta}_1$), while oracular selection clearly was the most accurate estimation method in most cases, the difference in accuracy between the estimation methods was modest in most cases. There were a few cases when the difference in MSE($\hat{\beta}_1$) between estimation methods amounted to at least an order of magnitude. At locations one and five of the parabola, oracular selection produces much more accurate estimation than GWEN, GWAL, or GWR because locations one and five are on the domain boundary where the parabola has a strong gradient, and those methods don't use locally linear

Data example: poverty rate in the upper midwest

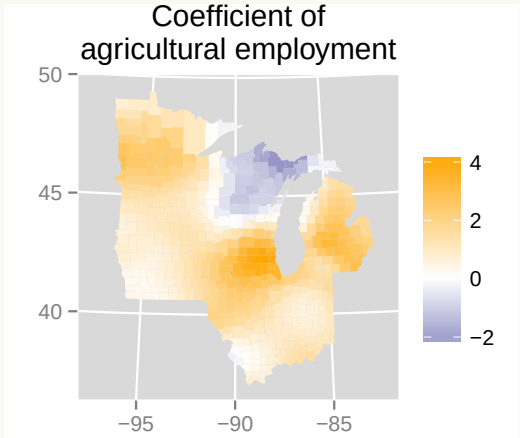
Data example: poverty rate in the upper midwest

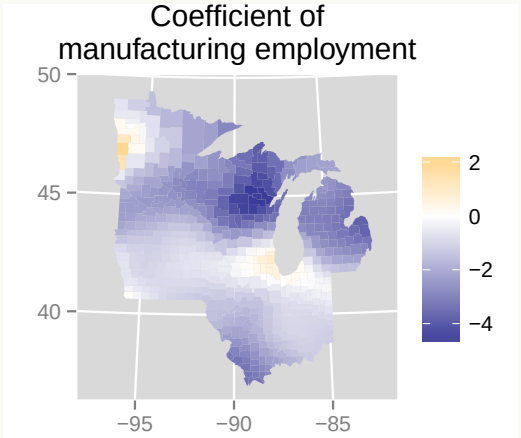
Revisiting the introductory example

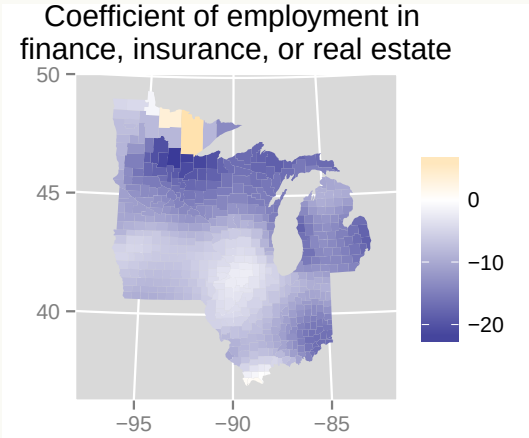


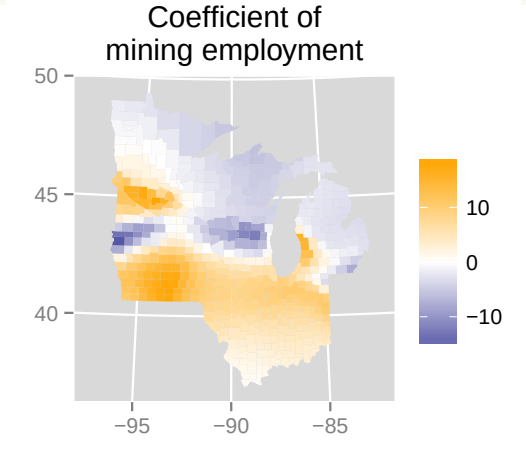
Data example: poverty rate in the upper midwest

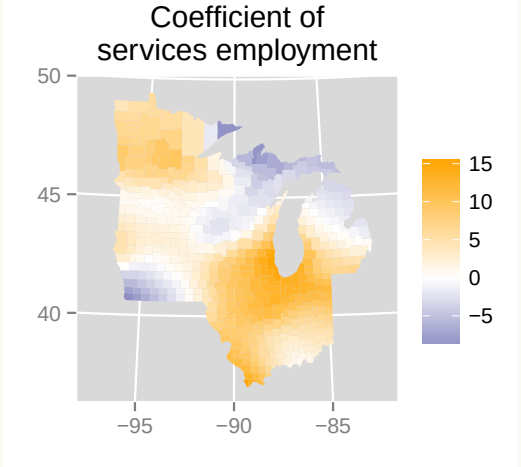
Results from traditional GWR

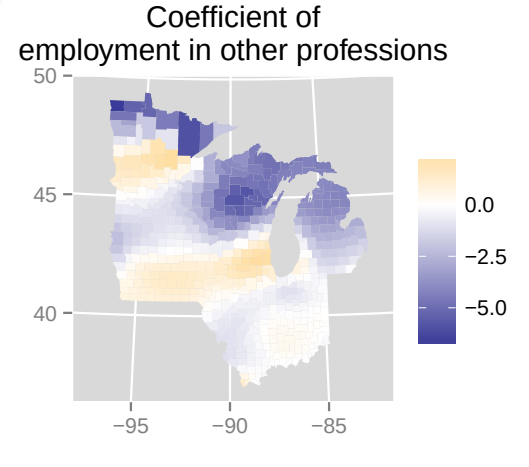












Data example: poverty rate in the upper midwest

Data description

- Response: logit-transformed poverty rate in the Upper Midwest states of the U.S.
  - Minnesota, Iowa, Wisconsin, Illinois, Indiana, Michigan
- Covariates: employment structure (raw proportion employed in:)
  - agriculture
  - finance, insurance, and real estate
  - manufacturing
  - mining
  - services
  - other professions
- Data source: U.S. Census Bureau's decennial census of 1970

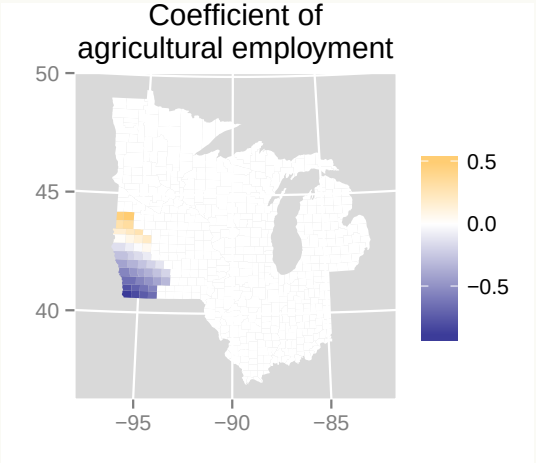
Data example: poverty rate in the upper midwest

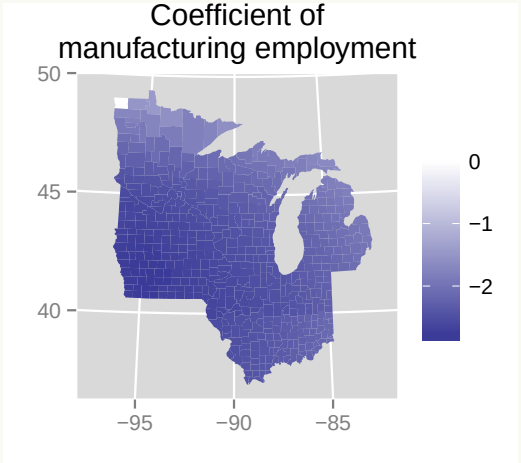
Data description

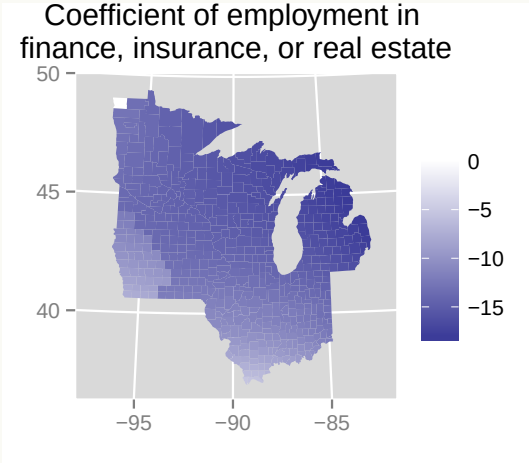
- Data aggregated to the county level
  - counties are areal units
- county centroid treated as sampling location

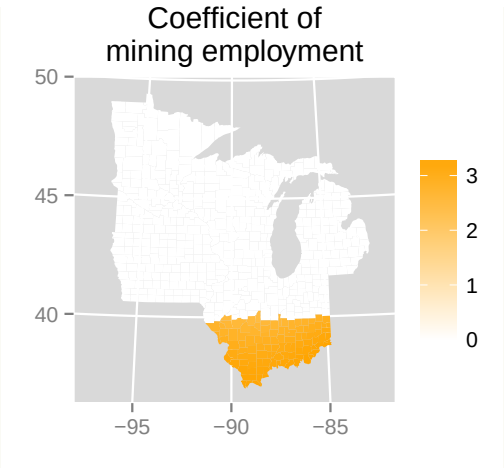
Data example: poverty rate in the upper midwest

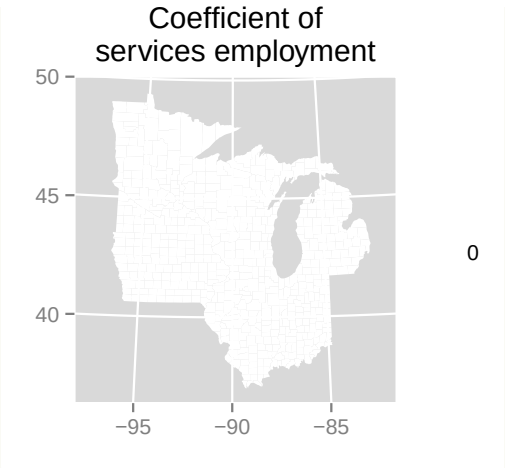
Results from GWEN











Data example: poverty rate in the upper midwest

Results from GWEN The coefficient surfaces estimated by the GWEN-LLE are relatively constant as compared to the those estimated by GWR. The GWEN-LLE indicates that the proportion of residents employed in services or in the ``other professions" category does not affect the poverty rate anywhere within the Upper Midwest states, while the proportion of residents employed in manufacturing or in finance, insurance, and real estate have negative coefficients (meaning a negative association with poverty rate) in all but one county of the Upper Midwest states (that one county is at the extreme northwest corner of Minnesota).
The coefficient of employment in finance, insurance, and real estate has a larger magnitude than the other covariates (minimum value near -20, as opposed to the next-largest-magnitude coefficient, that of manufacturing employment, with a minimum near -3), indicating that

Future work

Future work

- Apply the GWEN to data with non-Gaussian response variable
- Incorporate spatial autocorrelation in the model (simulated errors were iid)

Acknowledgements