# Local variable selection and parameter estimation for spatially varying coefficient models

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# Motivation

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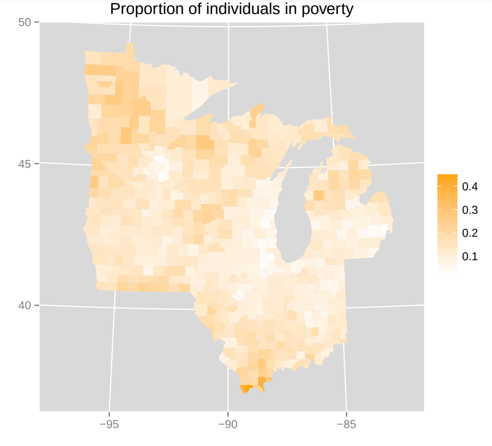
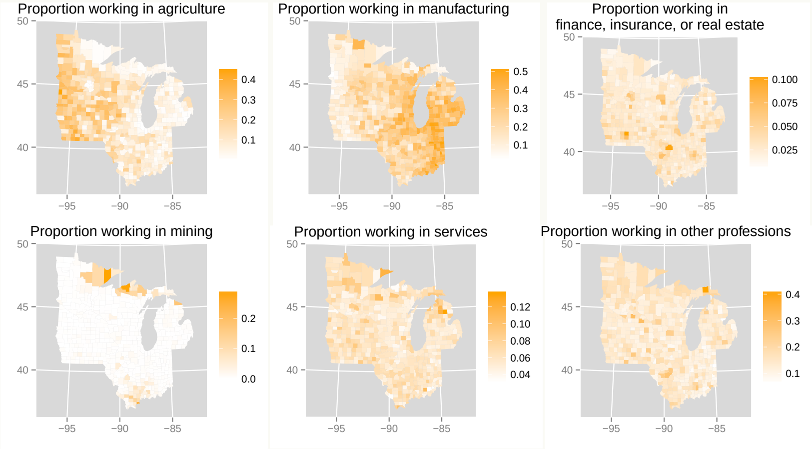
## Response variable



# Motivation

## Covariates



# Motivation

Scientific questions

- 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?
- How do the sign and magnitude of the associations vary across the region?

# Introduction

# Introduction

## An overview

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

# Introduction

## 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

## Types of spatial data

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

# Introduction

Spatial linear regression (Cressie, 1993)

- A typical spatial linear regression model

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

- $W(\boldsymbol{s})$ is a spatial random effect that accounts for autocorrelation in the response variable
- cov$(W(\boldsymbol{s}), W(\boldsymbol{t}))$: Matèrn class
- The coefficients $\boldsymbol{\beta} = (1, \beta_1, \ldots, \beta_p)$ are constant
- Relies on *a priori* global variable selection

# Introduction

Spatially varying coefficient model (Gelfand *et al.*, 2003)

- A more flexible model: coefficients in a spatial regression model can vary

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

- $\{\beta_0(\boldsymbol{s}) : \boldsymbol{s} \in \mathcal{D}\}, \ldots, \{\beta_p(\boldsymbol{s}) : \boldsymbol{s} \in \mathcal{D}\}$ are stationary spatial processes with Matèrn covariance functions
- Still relies on *a priori* global variable selection

# Introduction

Varying coefficients regression (VCR) (Hastie and Tibshirani, 1993)

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

- Assume an effect modifying variable $\boldsymbol{s}$
- Coefficients are functions of $\boldsymbol{s}$

# Introduction

Spline-based VCR models (Wood, 2006)

- Splines are a way to parameterize smooth functions
- Estimate the varying coefficients via splines:

$$E\{Y(t)\} = \beta_1(t)X_1(t) + \cdots + \beta_p(t)X_p(t)$$

Global selection in spline-based VCR models

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 (Wang *et al.*, 2008a)
  - Non-negative garrote penalty (Antoniadis *et al.*, 2012b)

# Introduction

Wavelet methods for VCR models

- Wavelet methods: decompose coefficient function into local frequency components
- Selection of nonzero local frequency components with nonzero coefficients:
  - Bayesian variable selection (Shang, 2011)
  - Lasso (Zhang and Clayton, 2011)
- Sparsity in the local frequency components; not in the local covariates

# Geographically weighted regression

# Geographically weighted regression

Brundson *et al.* (1998), Fotheringham *et al.* (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 $\varepsilon_i \overset{iid}{\sim} \mathcal{N}\left(0, \sigma^2\right)$

# Geographically weighted regression

Brundson *et al.* (1998), Fotheringham *et al.* (2002)

- The total log likelihood is

$$\ell\left(\boldsymbol{\beta}\right) = -\left(1/2\right)\left\{n \log\left(2\pi\sigma^2\right) + \sigma^{-2}\sum_{i=1}^{n}\left(y_i - \boldsymbol{x}_i'\boldsymbol{\beta}_i\right)^2\right\}$$

- With $n$ observations and $n(p+1)$ parameters, the model is not identifiable.
- Idea: to 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.

$$\mathcal{L}_i = \prod_{i'=1}^{n} \left(\mathcal{L}_{i'}\right)^{w_{ii'}}$$

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

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:

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

where

- $\phi$ is a bandwidth parameter
- $\delta_{ii'} = \delta(\boldsymbol{s}_i, \boldsymbol{s}_{i'}) = \|\boldsymbol{s}_i - \boldsymbol{s}_{i'}\|_2$ is the Euclidean distance between sampling locations $\boldsymbol{s}_i$ and $\boldsymbol{s}_{i'}$.

# Geographically weighted regression

Bandwidth estimation via the $AIC_c$ (Hurvich *et al.*, 1998)

- Smaller bandwidth: less bias, more flexible coefficient surface
- Large bandwidth: less variance, less flexible coefficient surface
- Choose the bandwidth parameter to optimize the bias-variance tradeoff

# Geographically weighted regression

Bandwidth estimation via the $\text{AIC}_c$ (Hurvich *et al.*, 1998)

- Idea: to estimate the degrees of freedom used in estmating the coefficient surface:
- Then the corrected AIC for bandwidth selection is:

$$\text{AIC}_c = 2n \log \sigma + n \left\{ \frac{n+\nu}{n-2-\nu} \right\}$$

  - $\hat{\boldsymbol{y}} = \boldsymbol{H}\boldsymbol{y}$
  - $\nu = \text{tr}(\boldsymbol{H})$
  - $\boldsymbol{H}_i = \left\{ \boldsymbol{W}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X} \right\}_i$
  - Where subscript $i$ indicates the $i$th row of the matrix

# Geographically weighted regression

Bandwidth estimation via GCV (Wahba, 1990)

- Idea: to estimate the degrees of freedom used in estmating the coefficient surface:
- Then the corrected AIC for bandwidth selection is:

$$GCV = \frac{\sum_i = 1^n \left(y - \hat{y}\right)^2}{(n - \nu)^2}$$

  - $\hat{\boldsymbol{y}} = \boldsymbol{H}\boldsymbol{y}$
  - $\nu =$ tr($\boldsymbol{H}$)
  - $\boldsymbol{H}_i = \left\{\boldsymbol{W}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}\right\}_i$
  - Where subscript $i$ indicates the $i$th row of the matrix

# Local variable selection and parameter estimation

# Geographically weighted Lasso

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 $s_i$ 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 elastic net (GWEN)

- Local variable selection in a GWR model using the adaptive elastic net (AEN) (Zou and 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)

- The AEN penalty function is

$$\mathcal{J}_2(\boldsymbol{\beta}_i) = \alpha_i \lambda_i^* \sum_{j=1}^{p} |\beta_{ij}|/\gamma_{ij} + (1-\alpha_i)\lambda_i^* \sum_{j=1}^{p} (\beta_{ij}/\gamma_{ij})^2$$

# Local variable selection and parameter estimation

## Bandwidth parameter estimation

- Traditional GWR:
  - $\hat{\boldsymbol{y}} = \boldsymbol{H}\boldsymbol{y}$
  - So traditional GWR is a linear smoother
  - $\nu = \text{tr}(\boldsymbol{H})$ is the degrees of freedom for the model
- GWAL:
  - $\hat{\boldsymbol{y}} = \boldsymbol{H}^{\dagger}\boldsymbol{y} - \boldsymbol{T}^{\dagger}\boldsymbol{\gamma}$
- GWEN:
  - $\hat{\boldsymbol{y}} = \boldsymbol{H}^{*}\boldsymbol{y} + \boldsymbol{T}^{*}\boldsymbol{\gamma}$
- Neither GWEN nor GWAL is a linear smoother
  - df not equal to trace of projection matrix for GWAL, GWEN
- Solution: use GWEN or GWAL for selection then fit local model for the selected variables via traditional GWR
  - Now df $= \nu = \text{tr}(\boldsymbol{H})$

# Local variable selection and parameter estimation

## Locally linear coefficient estimation

- GWR, GWEN, GWAL: coefficients locally constant
  - as in Nadaraya-Watson kernel smoother
  - Leads to bias where there is a gradient at the boundary
- Solution: local polynomial modeling
  - First-order polynomial: locally linear coefficients
- Augment with covariate-by-location interactions
  - Two-dimensional
  - Augment with selected covariates only

# Simulation study

# Simulation study

Simulating covariates

- $30 \times 30$ grid on $[0,1] \times [0,1]$
- Five covariates $\tilde{X}_1, \ldots, \tilde{X}_5$
- Gaussian random fields:

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

- Colinearity: $\rho$

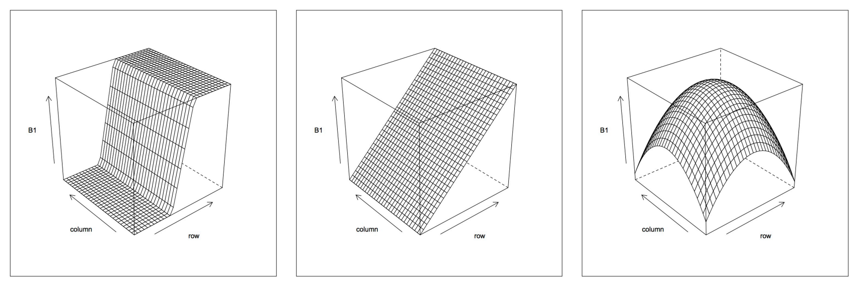
# Simulation study

## Simulating the response

- $Y(\boldsymbol{s}) = \boldsymbol{X}(\boldsymbol{s})'\boldsymbol{\beta}(\boldsymbol{s}) = \sum_{j=1}^{5} \beta_j(\boldsymbol{s}) X_j(\boldsymbol{s}) + \varepsilon(\boldsymbol{s})$
- $\varepsilon(\boldsymbol{s}) \sim \ iid \ \ N(0, \sigma^2)$
- $\beta_1(\boldsymbol{s})$, 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: step, gradient, and parabola



# Simulation study

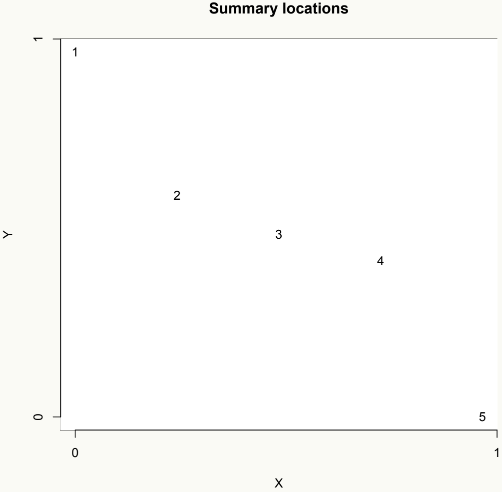
Simulation settings

Each setting simulated 100 times:

| Setting | function | $\rho$ | $\sigma^2$ |
|---|---|---|---|
| 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 |

# Simulation results

## Summary locations



# Simulation results

## Selection performance

- Non-ambiguous locations (80):
  - 52 saw no false negatives
  - 72 had no false positives
  - 26 neither false positives nor false negatives
- Incerased noise variance led to worse selection performance
- Increased colinearity in the covariates led to worse selection performance
- No difference between GWEN and GWAL

# Simulation results

Estimation performance

- Oracular selection
  - best MSE($\hat{\beta}_1$) in 41 of the 60 cases
- Generally small difference between GWR, oracular, GWEN-LLE, and GWAL-LLE
- Incerased noise variance led to worse estimation accuracy
- Increased colinearity in the covariates led to worse estimation accuracy
- Fitting $\hat{y}$: best MSE split between GWAL-LLE, oracle, and GWR

## Data example: poverty rate in the upper midwest

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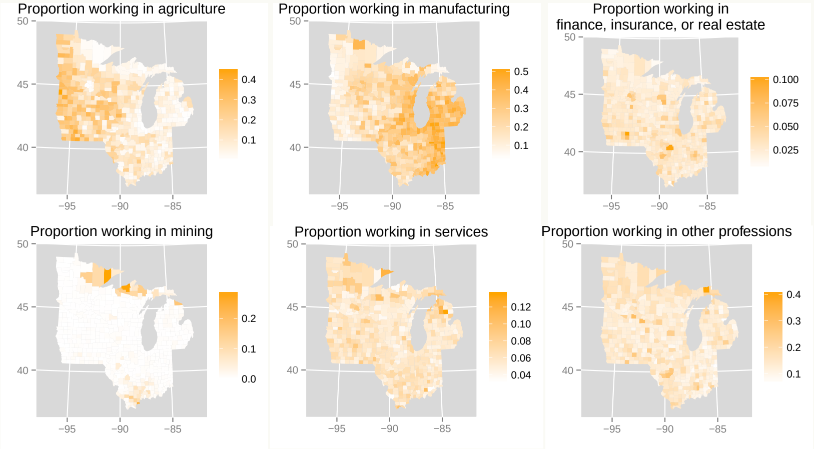
## Revisiting the motivating example



# 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

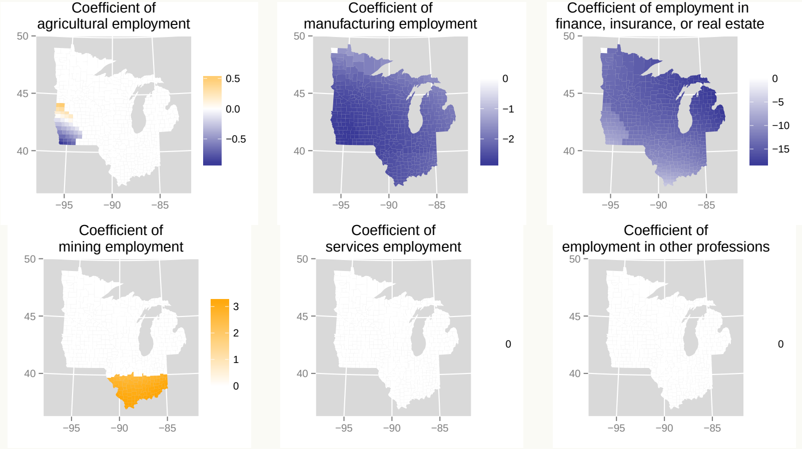
- Data aggregated to the county level
  - counties are areal units
- county centroid treated as sampling location

# Data example: poverty rate in the upper midwest

## Results from traditional GWR

# Data example: poverty rate in the upper midwest

## Results from GWEN



# Data example: poverty rate in the upper midwest

Results from GWEN-LLE

- Relatively constant compared to GWR
- Services, "other professions" do not affect the poverty rate
- Manufacturing: negative coefficient everywhere
- Finance, insurance, and real estate negative coefficient everywhere
  - Largest magnitude (min: -20, next-largest: -3)
  - GWR comparable to GWEN-LLE
- Manufacturing: negative coefficient everywhere
  - GWR: coefficient greater than zero near Chicago and in NW Minnesota
- Agriculture: nonzero in western Iowa
  - North-south gradient to coefficient
  - ranges positive to negative
- Mining: nonzero in parts south
  - Associated with increased poverty rate
  - Comparable to GWR within far southern range

# Future work

# Future work

- Apply the GWEN to models for non-Gaussian response variable
- Incorporate spatial autocorrelation in the model
- PalEON project: modeling and mapping tree biomass in the upper midwest

# Acknowledgements