Local variable selection and parameter estimation for spatially varying coefficient models

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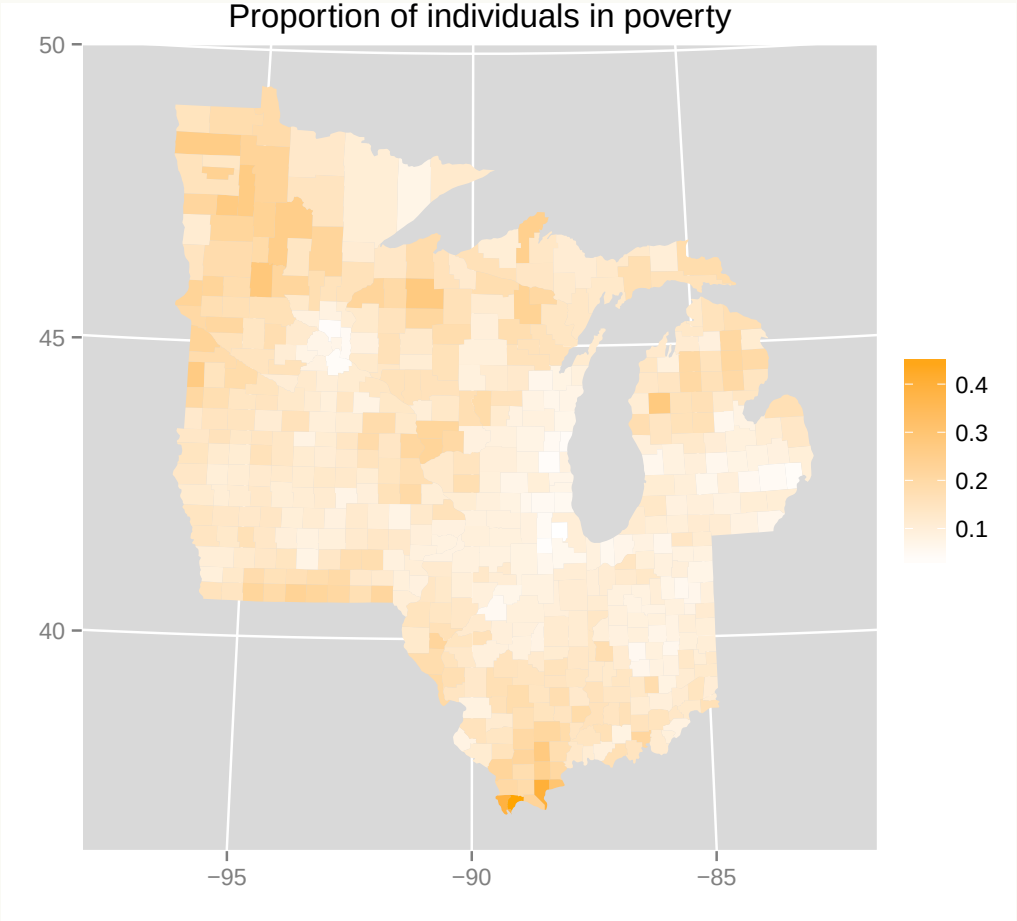
January 17, 2014

Motivation

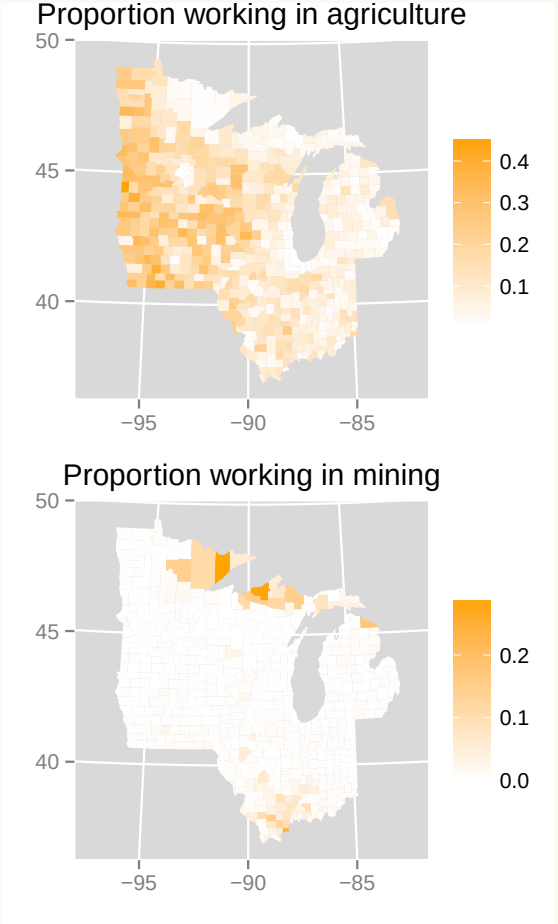
Motivation

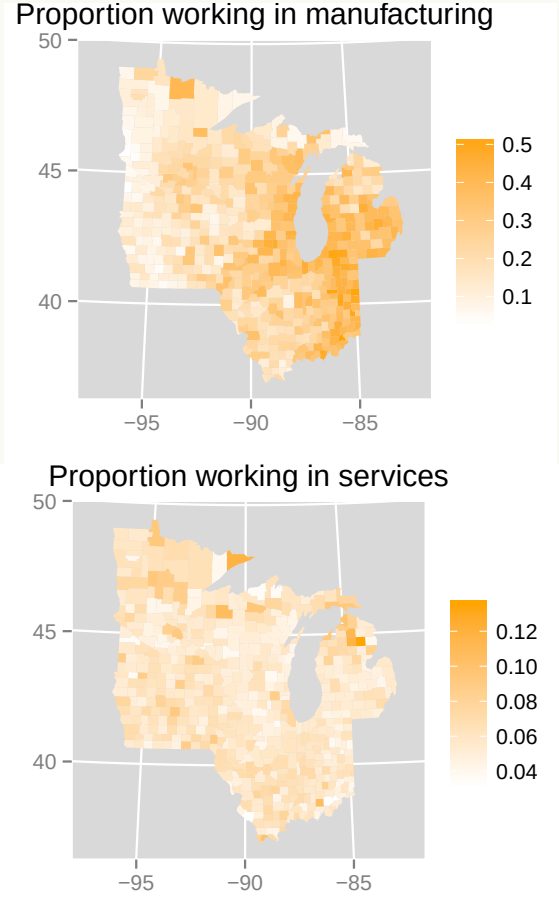
Response variable

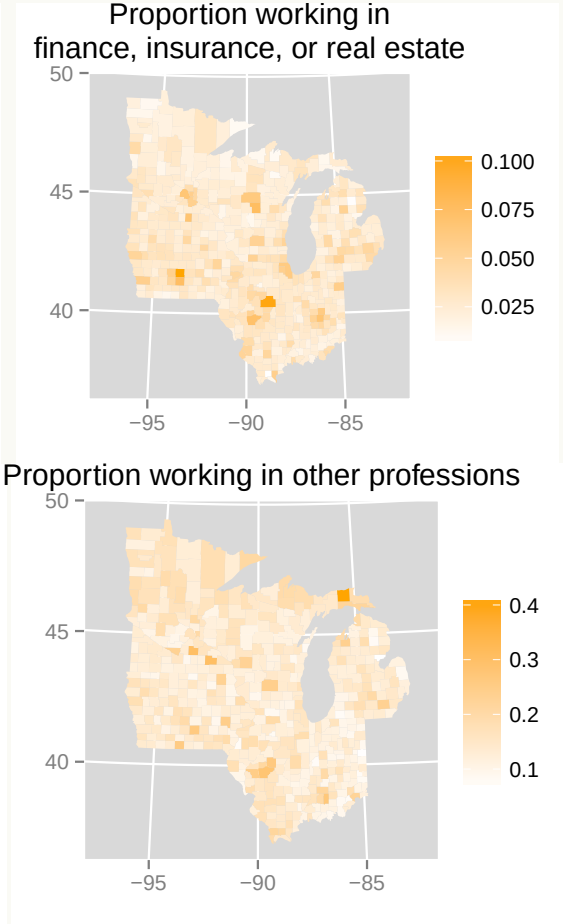


Motivation

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

- Definitions
- Spatial regression
- Varying coefficient regression
  - Splines
  - 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

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
- $\varepsilon(\boldsymbol{s})$ is iid random noise
- The coefficients $\boldsymbol{\beta} = (1, \beta_1, \ldots, \beta_p)$ are constant
- Requires *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
- Requires *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

Global selection in spline-based VCR models

Global variable selection can be done via regularization in a VCR model where the coefficient functions are modeled as splines

- The L_2 norm of a function (e.g. $\int \{f(t)\}^2 dt$) is zero if and only if the function is zero everywhere.
- Use regularization to penalize nonzero coefficient functions
  - SCAD penalty and B-splines (Wang *et al.*, 2008a)
  - Non-negative garrote penalty and P-splines (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-vector of covariates at location $\boldsymbol{s}_i$
- Assume $y_i = \boldsymbol{x}_i' \boldsymbol{\beta}_i + \varepsilon_i$ where $\varepsilon_i \overset{iid}{\sim} \mathcal{N}(0, \sigma^2)$

Geographically weighted regression

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

- The total log likelihood is

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

- With n observations and $np+1$ 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:

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

where

- ϕ 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 GCV (Wahba, 1990)

- The GCV criterion for bandwidth selection is:

$$\text{GCV} = \frac{\sum_{i=1}^{n} \left(y_i - \hat{y}_i\right)^2}{\left(n - \nu\right)^2}$$

  - $\hat{\boldsymbol{y}} = \boldsymbol{H}\boldsymbol{y}$
  - $\nu = \text{tr}(\boldsymbol{H})$
  - $\boldsymbol{H}_j = \left\{\boldsymbol{W}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}\right\}_j$
  - Where subscript j indicates the jth 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 $\boldsymbol{s}_i$ by minimizing a jacknife criterion: $|y_i - \hat{y}_i^{(-i)}|$
- 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
- Lasso not generally unbiased in variable selection (Fan and Li, 2001; Zou, 2006)

Local variable selection and parameter estimation

Geographically weighted adaptive elastic net (GWEN)

To overcome the shortcomings of the GWL, use a variable selection technique with potential for oracle properties and a tuning technique that can be applied anywhere on the domain.

- Local variable selection via the adaptive elastic net (AEN) (Zou and Zhang, 2009)
- Tuning parameters for local models selected by the BIC (Schwarz, 1978)

Local variable selection and parameter estimation

Geographically weighted adaptive elastic net (GWEN)

The adaptive elastic net:

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

Where

$$\boldsymbol{\gamma}_i = \left(\boldsymbol{X}'\boldsymbol{W}_i\boldsymbol{X}\right)^{-1} \boldsymbol{X}'\boldsymbol{W}_i\boldsymbol{Y}$$

Local variable selection and parameter estimation

Geographically weighted adaptive elastic net (GWAL)

- The adaptive Lasso penalty function is (Zou, 2006)

$$\mathcal{J}_1(\boldsymbol{\beta}_i) = \lambda_i \sum_{j=1}^{p} |\beta_{ij}|/|\gamma_{ij}|$$

- Under suitable conditions, the AL has an oracle property for selection in linear regression

Local variable selection and parameter estimation

Tuning parameter estimation

To estimate an AEN tuning parameter for each local model, use a local BIC that allows fitting a local model at any location within the spatial domain

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

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
- GWEN:
  - $\hat{\boldsymbol{y}} = \boldsymbol{H}^*\boldsymbol{y} - \boldsymbol{T}$
  - Where $T_i = \left\{ \boldsymbol{W}_i^{1/2}\boldsymbol{X}\left(\boldsymbol{X}'\boldsymbol{W}_i\boldsymbol{X} + (1-\alpha)\lambda I_p\right)^{-1}\frac{\lambda_i}{\gamma_i} \right\}_i$
- GWEN is not a linear smoother
- Solution: use GWEN for selection then fit local model for the selected variables via traditional GWR

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
  - Counter with locally linear coefficients
- Augment with covariate-by-location interactions:

$$Z_i = \left(\tilde{X}_i \;\; L_i \tilde{X}_i \;\; M_i \tilde{X}_i \right)$$

Where

- $\tilde{X}_i$ is the matrix of covariates selected for the model at location $\boldsymbol{s}_i$
- $L_i = \text{diag}\{s_{i',x} - s_{i,x}\}$ for $i' = 1, \ldots, n$
- $M_i = \text{diag}\{s_{i',y} - s_{i,y}\}$ for $i' = 1, \ldots, n$

Simulation study

Simulation study

Simulating covariates

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

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

- Colinearity: ρ
  - none ($\rho = 0$)
  - moderate ($\rho = 0.5$)

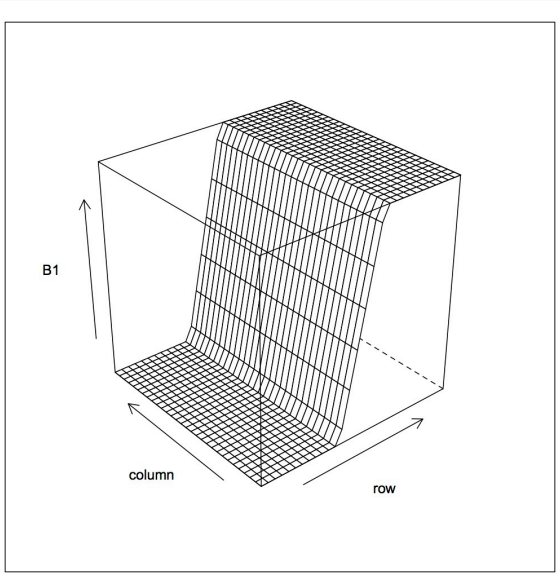
Simulation study

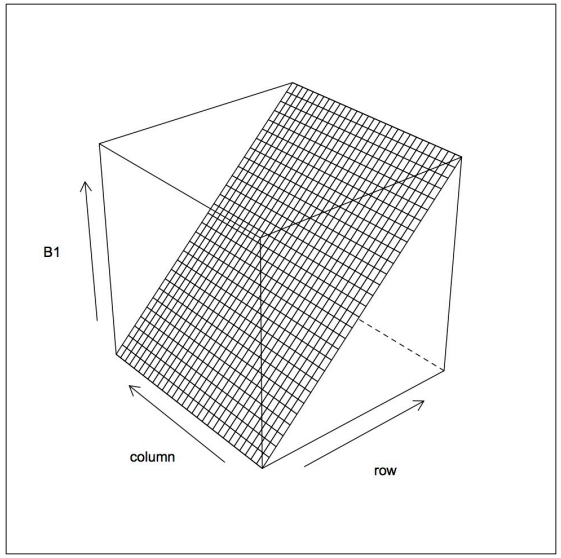
Simulating the response

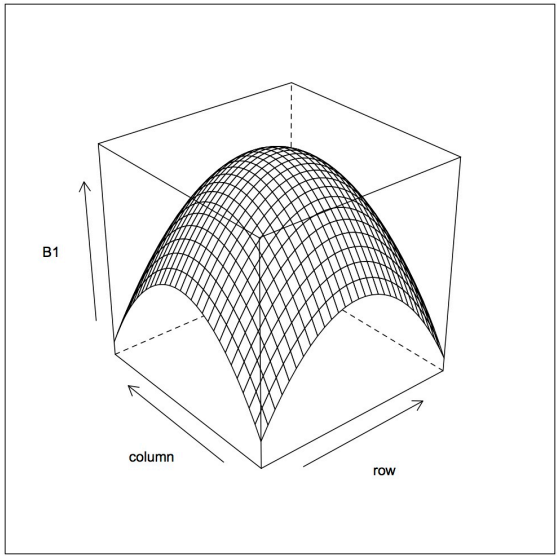
- $Y(\boldsymbol{s}) = \boldsymbol{X}(\boldsymbol{s})'\boldsymbol{\beta}(\boldsymbol{s}) = \sum_{j=1}^{5} \beta_j(\boldsymbol{s}) X_j(\boldsymbol{s}) + \varepsilon(\boldsymbol{s})$
- $\beta_1(\boldsymbol{s})$, the coefficient function for X_1, is nonzero in part of the domain.
- Coefficients for $X_2, \ldots, X_5$ are zero everywhere
- $\varepsilon(\boldsymbol{s}) \sim \ iid \ \ N(0, \sigma^2)$
  - Low noise: $\sigma = 0.5$
  - High noise: $\sigma = 1$

Simulation study

Coefficient functions: step, gradient, and parabola







Simulation study

Simulation settings

Each setting simulated 100 times:

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

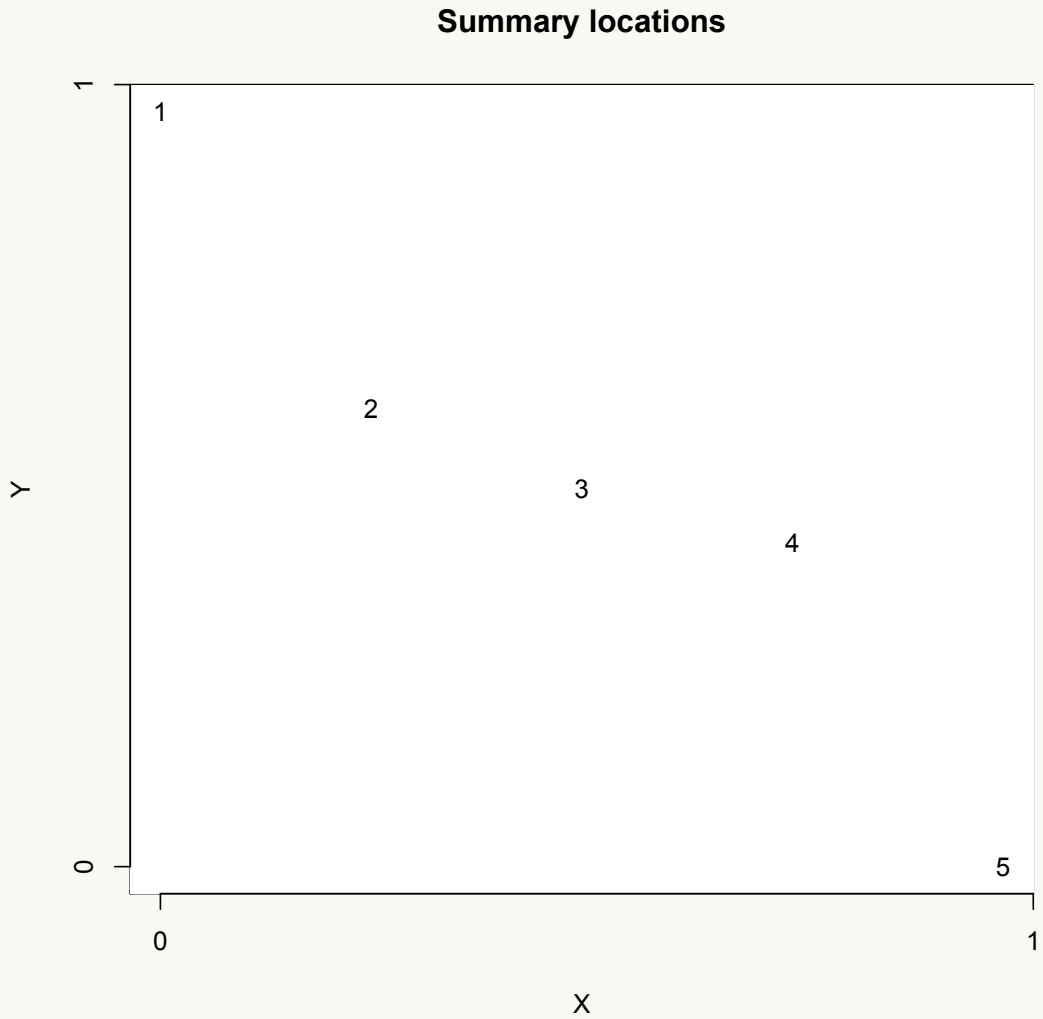
Simulation study

Estimation methods

method	selection	locally linear
GWR	NA	
oracular GWR	oracle	x
GWEN	GWEN	
GWAL	GWAL	
GWEN-LLE	GWEN	x
GWAL-LLE	GWAL	x

Simulation results

Summary locations



Simulation results

Selection performance

- GWEN selection (60 cases):
  - 21 with no false positives
  - 30 with no false negatives
  - 13 with neither
- GWAL selection (60 cases):
  - 27 with no false positives
  - 26 with no false negatives
  - 17 with neither
- Selection errors almost always below five percent
- Worst false positive rate: 8% at location three of the step function (GWEN selection)
- Worst false negative rate: 13% (same location, GWAL selection)
- No consistent difference between GWEN and GWAL

Simulation results

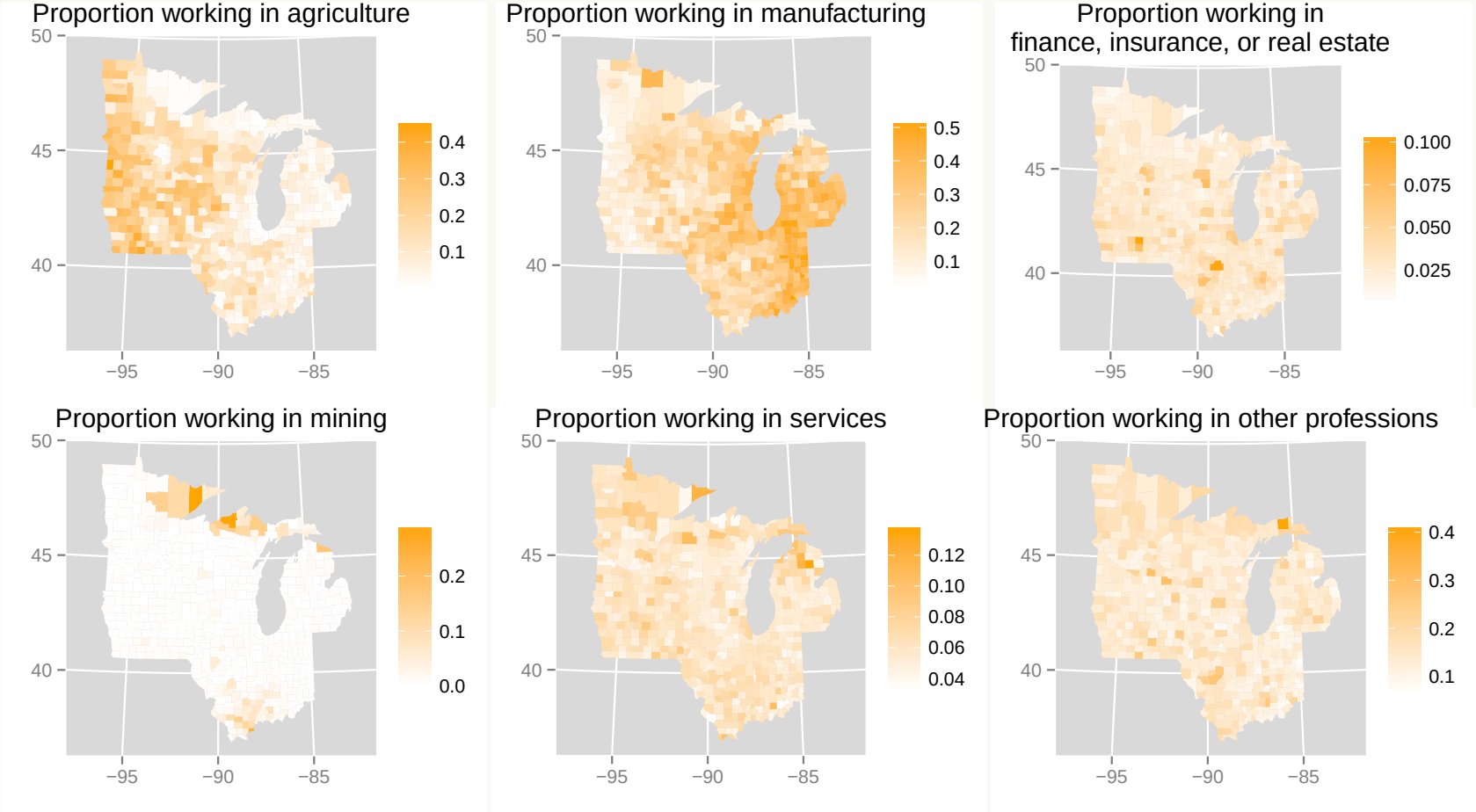
Estimation performance

- Cases where oracular GWR clearly had the best performance
  - Minimum MSE($\hat{\beta}_1$): 38 of 60
  - Minimum var($\hat{\beta}_1$): 44 of 60
- Generally small differences between GWR, oracular GWR, GWEN-LLE, and GWAL-LLE
- Methods with locally constant coefficients had larger bias at the boundaries
- Fitting $\hat{y}$: MSE nearest σ^2 split between GWAL-LLE, oracle, and GWR

Data example: poverty rate in the upper midwest

Data example: poverty rate in the upper midwest

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

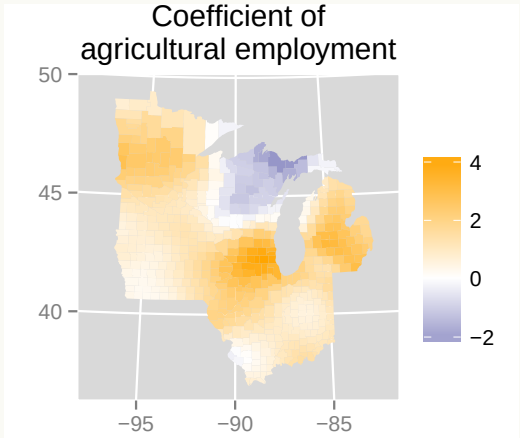
Data example: poverty rate in the upper midwest

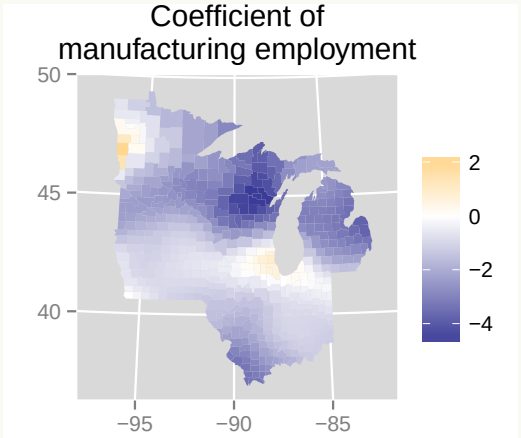
Data description

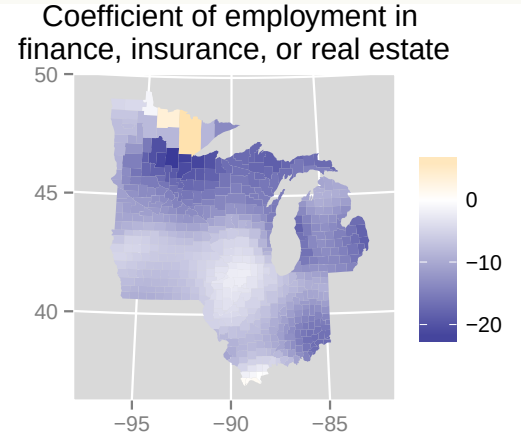
- Data aggregated to the county level
  - counties are areal units
- county centroid treated as sampling location

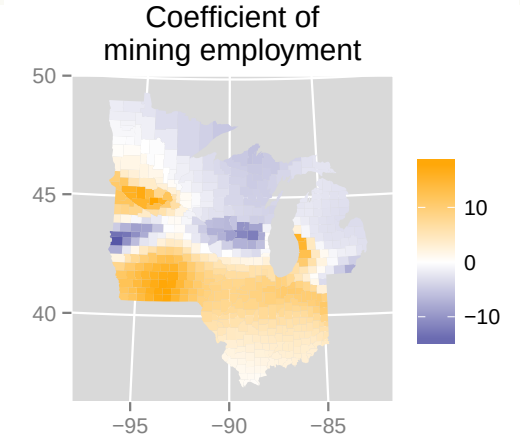
Data example: poverty rate in the upper midwest

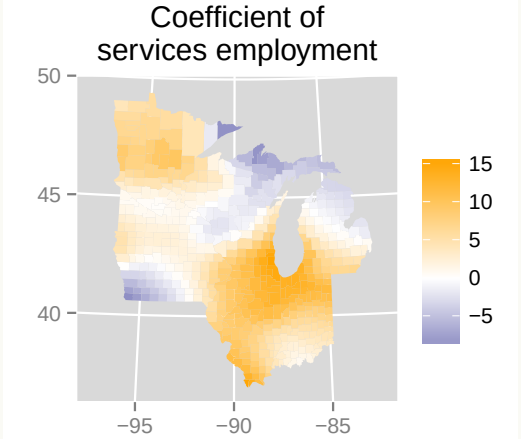
Results from traditional GWR

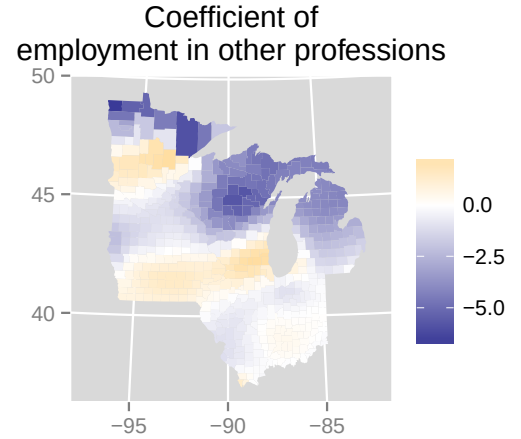






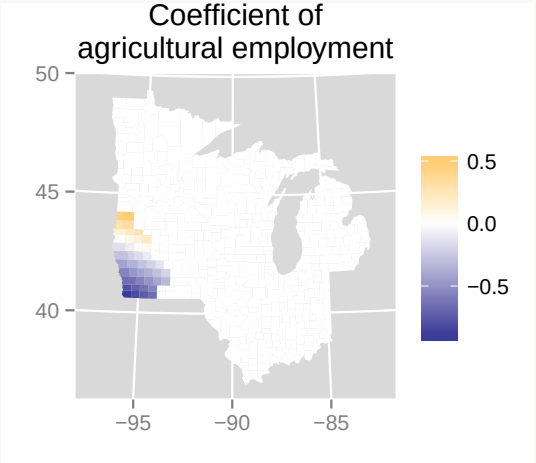


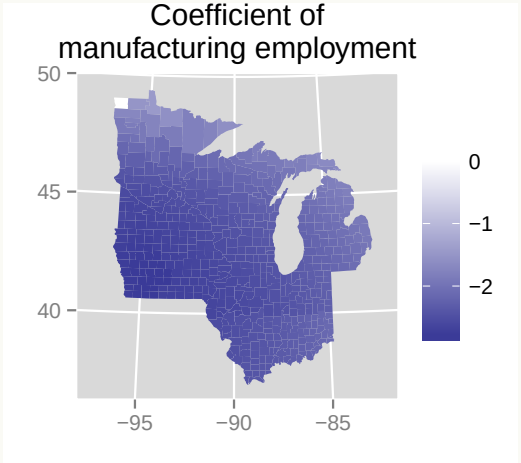


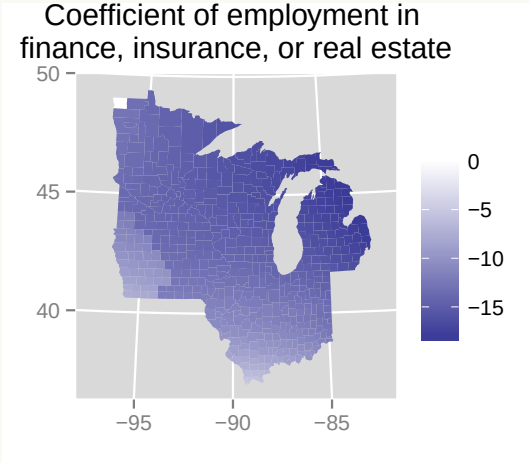


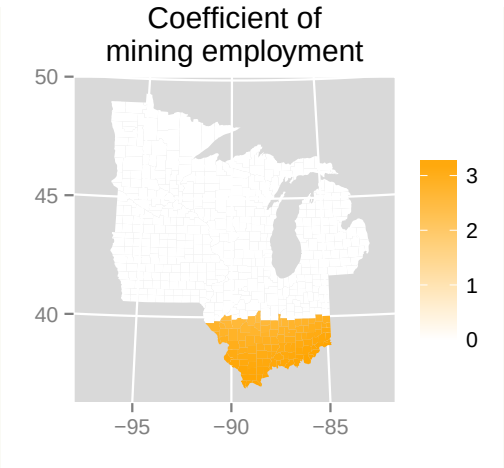
Data example: poverty rate in the upper midwest

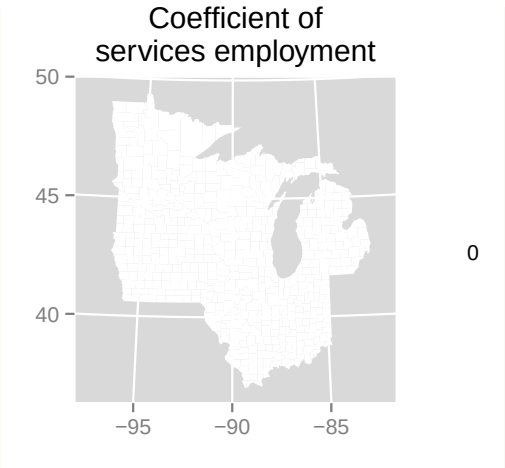
Results from GWEN





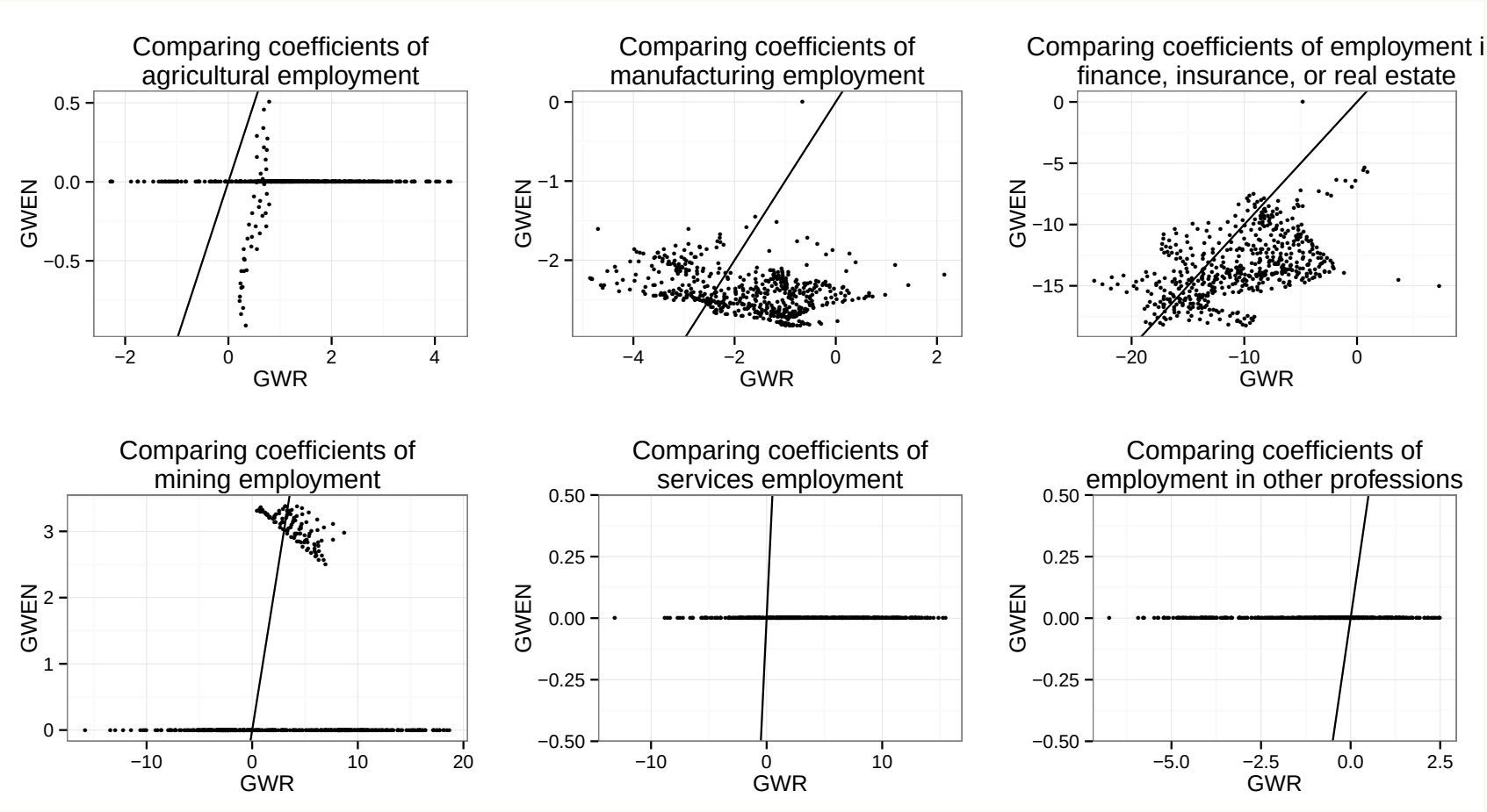






Data example: poverty rate in the upper midwest

Comparing the coefficients from GWR and the GWEN



Data example: poverty rate in the upper midwest

Results from GWEN-LLE

- Relatively constant compared to GWR
- Not associated with poverty rate: Services, "other professions" sector
- 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
- Investigate the asymptotic properties of the GWEN
- Incorporate spatial autocorrelation in the model
- PalEON project: modeling and mapping tree biomass in the upper midwest

Thank you!